

Product Name: Verubecestat

Catalog No.: 7659

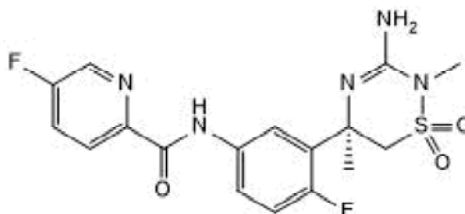
Batch No.: 1

CAS Number: 1286770-55-5

IUPAC Name: *N*-[3-[(5*R*)-3-Amino-5,6-dihydro-2,5-dimethyl-1,1-dioxido-2*H*-1,2,4-thiadiazin-5-yl]-4-fluorophenyl]-5-fluoro-2-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₁₇ H ₁₇ F ₂ N ₅ O ₃ S
Batch Molecular Weight:	409.41
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 20 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.4% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Optical Rotation:	[α] _D = +37.3 (Concentration = 0.367, Solvent = Methanol)
Microanalysis:	
	Carbon Hydrogen Nitrogen
	Theoretical 49.87 4.19 17.11
	Found 49.94 4.2 17.01

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Verubecestat is a high affinity and selective β -secretase 1 (BACE1) and its homolog BACE2 inhibitor (K_i of 2.2 nM and 0.38 nM respectively). It exhibits no inhibition of cathepsin D, cathepsin E, pepsin, or renin. Verubecestat potently reduces A β 40 formation in HEK293 APP^{Swe/Lon} cells (IC_{50} = 2.1 nM). Verubecestat significantly lowers CSF and brain A β levels in rats. Orally bioavailable.

Physical and Chemical Properties:

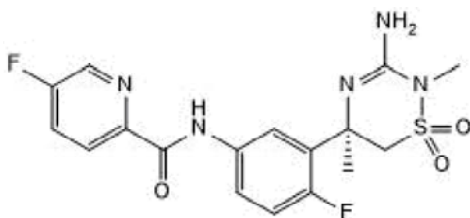
Batch Molecular Formula: C₁₇H₁₇F₂N₅O₃S.

Batch Molecular Weight: 409.41

Physical Appearance: White solid

Minimum Purity: \geq 98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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:

Scott *et al* (2016) Discovery of the 3-imino-1,2,4-thiadiazinane 1,1-dioxide derivative Verubecestat (MK-8931) - A β -site amyloid precursor protein cleaving enzyme 1 inhibitor for the treatment of Alzheimer's disease. *J.Med.Chem.* **59** 10435. PMID: 27933948.

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