

**Product Name:** LY 450139

**Catalog No.:** 6559

**Batch No.:** 1

CAS Number: 425386-60-3

IUPAC Name: (2*S*)-2-Hydroxy-3-methyl-*N*-[(1*S*)-1-methyl-2-oxo-2-[[[(1*S*)-2,3,4,5-tetrahydro-3-methyl-2-oxo-1*H*-3-benzazepin-1-yl]amino]ethyl]butanamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>27</sub>N<sub>3</sub>O<sub>4</sub>·¼H<sub>2</sub>O

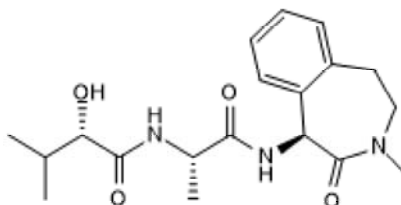
**Batch Molecular Weight:** 365.94

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.36	7.57	11.48
Found	62.15	7.63	11.17

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

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**Description:**

γ-secretase pseudo-inhibitor. Inhibits Aβ secretion from cells in vitro and increases accumulation of γ-secretase products and long Aβ species in vitro and in vivo. Also attenuates the accumulation of activated microglia and neurological injury in a traumatic brain injury animal model.

**Physical and Chemical Properties:**

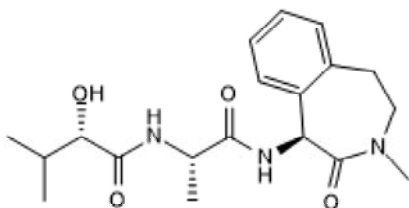
Batch Molecular Formula: C<sub>19</sub>H<sub>27</sub>N<sub>3</sub>O<sub>4</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 365.94

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol 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:**

**Lin et al** (2017) Gamma-secretase inhibitors attenuate neurotrauma and neurogenic acute lung injury in rats by rescuing the accumulation of hypertrophic microglia. *Cell Physiol.Biochem.* **44** 1726. PMID: 29227981.

**Tagami et al** (2017) Semagacestat is a pseudo-inhibitor of γ-secretase. *Cell Rep.* **21** 259. PMID: 28978478.

**Henley et al** (2009) Development of semagacestat (LY450139), a functional gamma-secretase inhibitor, for the treatment of Alzheimer's disease. *Expert Opin.Pharmacother.* **10** 1657. PMID: 19527190.

**Lanz et al** (2006) Concentration-dependent modulation of amyloid-beta *in vivo* and *in vitro* using the gamma-secretase inhibitor, LY-450139. *J.Pharmacol.Exp.Ther.* **319** 924. PMID: 16920992.

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