

Product Name: Compound E

Catalog No.: 6476

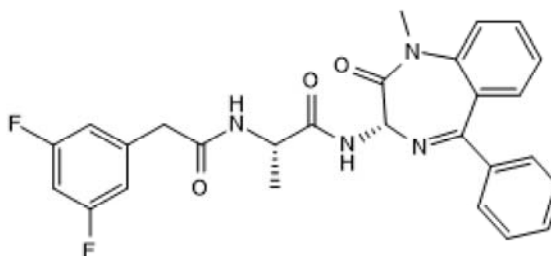
Batch No.: 4

CAS Number: 209986-17-4

IUPAC Name: *N*-[(1*S*)-2-[[[(3*S*)-2,3-Dihydro-1-methyl-2-oxo-5-phenyl-1*H*-1,4-benzodiazepin-3-yl]amino]-1-methyl-2-oxoethyl]-3,5-difluorobenzeneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₄F₂N₄O₃
Batch Molecular Weight: 490.5
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.39 (Ethyl acetate:Petroleum ether [4:1])
HPLC: Shows 99.8% purity
Chiral HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.11	4.93	11.42
Found	65.95	4.92	11.41

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

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Description:

γ-secretase inhibitor. Enhances growth inhibition, differentiation and migration of neuroblastoma cells when used in a combination with DAPT (Cat. No. 2634) and 13-cis RA. In combination with hLIF, CHIR 99021 (Cat. No. 4423) and SB 431542 (Cat.No. 1614), accelerates the induction of a homogeneous, self-renewing primitive neuroepithelium population from hESCs. Active in vitro and in vivo.

Physical and Chemical Properties:

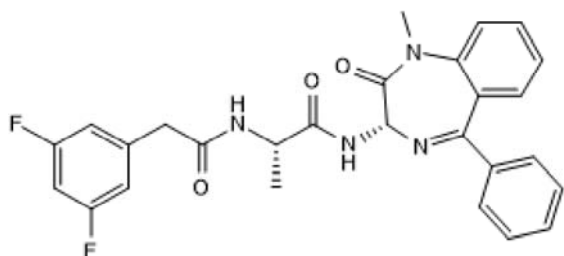
Batch Molecular Formula: C₂₇H₂₄F₂N₄O₃

Batch Molecular Weight: 490.5

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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.

Other Information:

INFORMATION FOR CUSTOMERS IN CANADA ONLY

This product is a Schedule IV CDSA controlled substance and customers in Canada require an import permit to purchase this material.

References:

Li *et al* (2011) Rapid induction and long-term self-renewal of primitive neural precursors from human embryonic stem cells by small molecule inhibitors. *Proc.Natl.Acad.Sci.USA* **108** 8299. PMID: 21525408.

Ferrari-Toninelli *et al* (2010) Targeting Notch pathway induces growth inhibition and differentiation of neuroblastoma cells. *Neuro.Oncol.* **12** 1231. PMID: 20716592.

Behr *et al* (2001) Pharmacological knock-down of the presenilin 1 heterodimer by a novel gamma -secretase inhibitor: implications for presenilin biology. *J.Biol.Chem.* **276** 45394. PMID: 11574530.

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