

# Certificate of Analysis

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### Product Name: MRK 560

Catalog No.: 4000 Batch No.: 1

 CAS Number:
 677772-84-8

 IUPAC Name:
 N-[cis-4-[(4-Chlorophenyl)sulfonyl]-4-(2,5-difluorophenyl)cyclohexyl]-1,1,1-trifluoromethanesulfonamide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Storage: Batch Molecular Structure: C<sub>19</sub>H<sub>17</sub>CIF<sub>5</sub>NO<sub>4</sub>S<sub>2</sub> 517.92 White solid DMSO to 100 mM ethanol to 50 mM Store at +4°C

CI SO2 F<sub>2</sub>C

# 2. ANALYTICAL DATA

TLC: HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: R<sub>f</sub> = 0.4 (Chloroform/Ethyl acetate [95:5]) Shows 100% purity Consistent with structure Consistent with structure

	Carbon	Hydrogen	Nitrogen
Theoretical	44.06	3.31	2.7
Found	44.15	3.3	2.82

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





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#### **Description:**

**IUPAC Name:** 

 $\gamma$ -secretase inhibitor; inhibits proteolytic cleavage of amyloid precursor protein (APP) over the Notch pathway. Reduces levels of A $\beta$  in the brain (inhibits A $\beta$ 40 and A $\beta$ 42 in SH-SY5Y neuroblastoma cells with an IC<sub>50</sub> of 0.65 nM); attenuates plaque deposition. Orally bioavailable.

#### **Physical and Chemical Properties:**

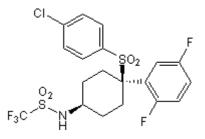
Batch Molecular Formula: C<sub>19</sub>H<sub>17</sub>CIF<sub>5</sub>NO<sub>4</sub>S<sub>2</sub>

Batch Molecular Weight: 517.92

Physical Appearance: White solid

#### Minimum Purity: >99%

#### **Batch Molecular Structure:**



#### Storage: Store at +4°C

#### Solubility & Useage 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  $45-60^{\circ}$ C water bath).

Catalog No.: 4000

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:**

**Best** *et al* (2006) In vivo characterization of A $\beta$ (40) changes in brain and cerebrospinal fluid using the novel  $\gamma$ -secretase inhibitor *N*-[*cis*-4-[(4-chlorophenyl)sulfonyl]-4-(2,5-difluorophenyl)cyclohexyl]-1,1,1-trifluoromethanesulfonamide (MRK-560) in the rat. J.Pharm.Exp.Ther. **317** 786. PMID: 16443723.

**Best** *et al* (2007) The novel  $\gamma$ -secretase inhibitor *N*-[*cis*-4-[(4-chlorophenyl)sulfonyl]-4-(2,5-difluorophenyl)cyclohexyl]-1,1,1-trifluoromethanesulfonamide (MRK-560) reduces amyloid plaque deposition without evidence of Notch-related pathology in the Tg2576 mouse. J.Pharm.Exp.Ther. **320** 552. PMID: 17099072.

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