

**Product Name:** Aliskiren hemifumarate

**Catalog No.:** 5491

**Batch No.:** 1

CAS Number: 173334-58-2

IUPAC Name: ( $\alpha$ S, $\gamma$ S, $\delta$ S, $\zeta$ S)- $\delta$ -Amino-N-(3-amino-2,2-dimethyl-3-oxopropyl)- $\gamma$ -hydroxy-4-methoxy-3-(3-methoxypropoxy)- $\alpha$ , $\zeta$ -bis(1-methylethyl)benzeneoctanamide hemifumarate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>30</sub>H<sub>53</sub>N<sub>3</sub>O<sub>6</sub>. 1/2C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>. 1/2H<sub>2</sub>O

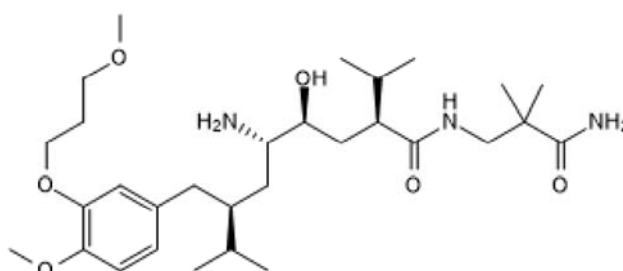
**Batch Molecular Weight:** 618.84

**Physical Appearance:** White solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



1/2 C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

## 2. ANALYTICAL DATA

**HPLC:** Shows 99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	62.11	9.12	6.79
Found	61.99	9.13	6.83

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

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**Description:**

Potent renin inhibitor (IC<sub>50</sub> = 0.6 and 80 nM for human and rat respectively). Exhibits selectivity for renin over a range of other aspartic proteinases (>5000 nM). Lowers blood pressure in a hypertensive rodent model. Orally active.

**Physical and Chemical Properties:**

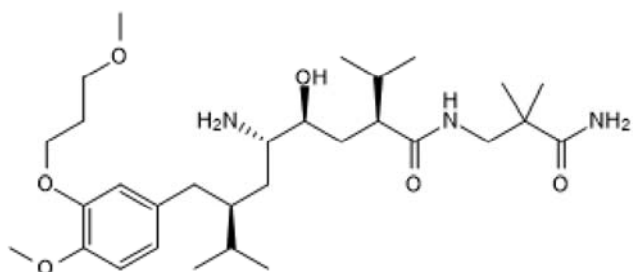
Batch Molecular Formula: C<sub>30</sub>H<sub>53</sub>N<sub>3</sub>O<sub>6</sub>.1/2C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.1/2H<sub>2</sub>O

Batch Molecular Weight: 618.84

Physical Appearance: White solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**



1/2 C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 100 mM

DMSO 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:**

**Kaye and Krum** (2007) Drug discovery for heart failure: a new era or the end of the pipeline? *Nat.Rev.Drug Discov.* **6** 127. PMID: 17268484.

**Jensen et al** (2) Aliskiren: the first renin inhibitor for clinical treatment. *Nat.Rev.Drug Discov.* **7** 399. PMID: 18340340.

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