

**Product Name:** A 410099.1

**Catalog No.:** 6470

**Batch No.:** 1

CAS Number: 762274-58-8

IUPAC Name: *N*-Methyl-L-alanyl-(2*S*)-2-cyclohexylglycyl-*N*-[(1*R*)-1,2,3,4-tetrahydro-1-naphthalenyl]-L-prolinamide hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>40</sub>N<sub>4</sub>O<sub>3</sub>·HCl·½H<sub>2</sub>O

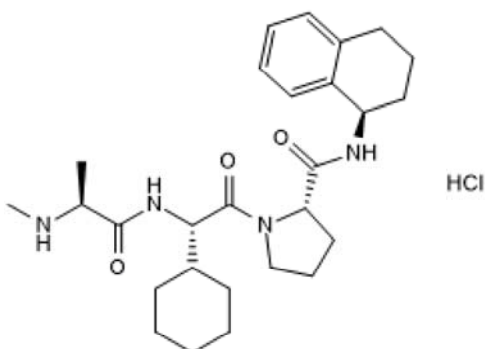
**Batch Molecular Weight:** 514.1

**Physical Appearance:** White solid

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

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.19 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99.3% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.08	8.23	10.9
Found	63.16	8.29	10.97

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**Description:**

High affinity XIAP antagonist ( $K_d = 16$  nM for the BIR3 domain of XIAP). Exhibits cytotoxicity in a wide range of cancer cell lines in vitro ( $EC_{50} = 13$  nM in MDA-MB-231 cells). Also displays antitumor activity in a mouse breast cancer xenograft model. Enhances TRAIL-induced apoptosis in chronic lymphocytic leukemia (CLL) cells.

**Physical and Chemical Properties:**

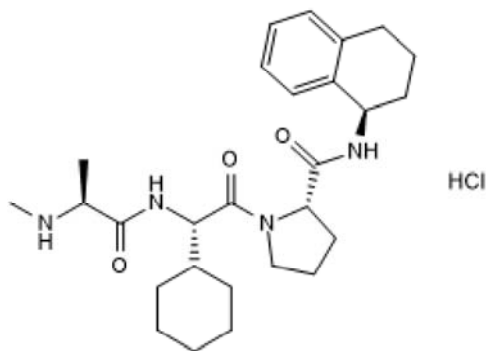
Batch Molecular Formula:  $C_{27}H_{40}N_4O_3 \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 514.1

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 100 mM  
DMSO to 100 mM  
ethanol 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:**

**Loeder *et al*** (2009) A novel paradigm to trigger apoptosis in chronic lymphocytic leukemia. *Cancer Res.* **69** 8977. PMID: 19920200.

**Oost *et al*** (2004) Discovery of potent antagonists of the antiapoptotic protein XIAP for the treatment of cancer. *J.Med.Chem.* **47** 4417. PMID: 15317454.

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