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Print Date: Jan 14th 2019

# Certificate of Analysis

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**Product Name:** **L 006235** **Catalog No.: 3066** **Batch No.: 3**

CAS Number: 294623-49-7

IUPAC Name: *N*-[1-[[(Cyanomethyl)amino]carbonyl]cyclohexyl]-4-[2-(4-methyl-1-piperazinyl)-4-thiazolyl]benzamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{24}H_{30}N_6O_2S$

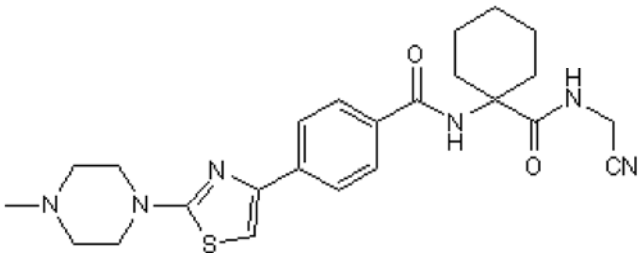
**Batch Molecular Weight:** 466.6

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.29 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 98.8% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 61.78 | 6.48 | 18.01 |
| Found | 61.6 | 6.43 | 17.9 |



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# Product Information



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IUPAC Name: *N*-[1-[[(Cyanomethyl)amino]carbonyl]cyclohexyl]-4-[2-(4-methyl-1-piperazinyl)-4-thiazolyl]benzamide

**Description:**

Potent, reversible cathepsin K inhibitor ($IC_{50}$ = 0.25 nM) that displays > 4000-fold selectivity over cathepsins B, L and S. Displays reduced selectivity in cell-based assays possibly due to lysosomal accumulation. Reduces collagen breakdown and promotes bone deposition in vivo. Orally active and has intrinsic fluorescence.

**Physical and Chemical Properties:**

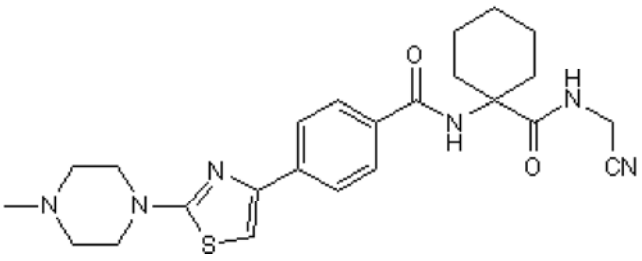
Batch Molecular Formula: $C_{24}H_{30}N_6O_2S$

Batch Molecular Weight: 466.6

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Usage Info:**

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:**

**Desmarais** *et al* (2008) Effects of cathepsin K inhibitors basicity on in vivo off-target activities. Mol.Pharmacol. ***73*** 147. PMID: 17940194.

**Falgueyret** *et al* (2005) Lysosomotropism of basic cathepsin K inhibitors contributes to increased cellular potencies against off-target cathepsins and reduced functional selectivity. J.Med.Chem. ***48*** 7535. PMID: 16302795.

**Palmer** *et al* (2005) Design and synthesis of tri-ring $P_3$ benamide-containing aminonitriles as potent, selective, orally effective inhibitors of cathepsin K. J.Med.Chem. ***48*** 7520. PMID: 16302794.