

Certificate of Analysis

Print Date: Oct 12th 2022

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Product Name: Balicatib Catalog No.: 5585 Batch No.: 1

CAS Number: 354813-19-7

IUPAC Name: N-[1-(Cyanomethylcarbamoyl)cyclohexyl]-4-(4-propylpiperazin-1-yl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{33}N_5O_2$ Batch Molecular Weight:411.54Physical Appearance:White solid

Solubility: DMSO to 100 mM

ethanol to 10 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.19 8.08 17.02 Found 66.97 7.99 16.93



Product Information

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Description:

Balicatib is a potent and selective cathepsin K inhibitor (IC_{50} values are 1.4, 56 and 480 nM for human, rat and mouse cathepsin K, respectively). Exhibits >300-fold selectivity for cathepsin K over cathepsins L, B and S. Long term supratherapeutic dosing increases tissue levels of cathepsins L and B in rats.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₃₃N₅O₂ Batch Molecular Weight: 411.54 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

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) Effect of cathepsin k inhibitor basicity on in vivo off-target activities. Mol. Pharmacol. 73 147. PMID: 17940194.