

Certificate of Analysis

Print Date: Feb 13th 2023

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Product Name: NR 162 Catalog No.: 7572 Batch No.: 1

CAS Number: 2755241-73-5

IUPAC Name: 4-(Cyclopentylamino)-2-((2,5-dibromo-4-methylbenzyl)amino)-*N*-(3-(2-oxooxazolidin-3-yl)propyl)pyrimidine-5-

carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{30}Br_2N_6O_3$

Batch Molecular Weight: 610.35 **Physical Appearance:** White solid

Solubility: DMSO to 20 mM

ethanol to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.23 4.95 13.77 Found 47.24 4.86 13.61

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Product Information

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Description:

NR 162 is a potent and selective calcium/calmodulin-dependent serine protein kinase (CASK) inhibitor (IC $_{50}$ = 80 nM); it exhibits no significant activity against related kinases MERTK, AXL and ABL1 and ~ 47-fold selectivity over TYRO3 (IC $_{50}$ = 3.8 μ M). NR 162 targets the unique pocket created by CASK GFG motif; it is a type-I inhibitor which stabilizes the active state of CASK without affecting the scaffolding function. NR 162 induces cell death in actively differentiating cells of the P19 neuronal differentiation model. NR 162 shows no toxicity in differentiated cells, or in cancer cells.

Physical and Chemical Properties:

Batch Molecular Formula: C24H30Br2N6O3

Batch Molecular Weight: 610.35 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM ethanol to 5 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the NR 162 probe summary on the SGC website.

References:

Russ et al (2021) Design and development of a chemical probe for pseudokinase Ca²⁺/calmodulin-dependent Ser/Thr kinase. J.Med.Chem. **64** 14358, PMID: 34543009.

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