Certificate of Analysis

Product Name: **NCL 00017509** **Catalog No.: 5150** **Batch No.: 1**

CAS Number: 1507367-00-1

IUPAC Name: 3-[(6-Ethynyl-9*H*-purin-2-yl)amino]benzeneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{12}N_6O.¾H_2O$

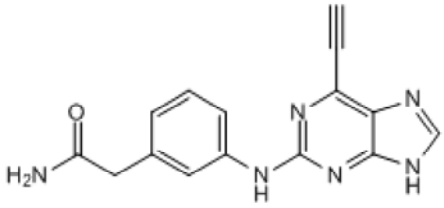
Batch Molecular Weight: 305.81

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Dichloromethane:Methanol [9:1])

HPLC: Shows 97.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.91	4.45	27.48
Found	58.89	4.21	27.52

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Description:

NCL 00017509 is a potent and reversible NIMA related kinase 2 (Nek2) inhibitor (IC_{50} = 56 nM). Induces increased mitotic abnormalities and mitotic delay. Cell permeable and active in vivo. In mice bearing pancreatic tumors, NCL 00017509 decreases PD-L1 expression and induces an anticancer immune response.

Physical and Chemical Properties:

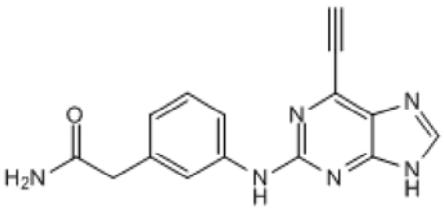
Batch Molecular Formula: $C_{15}H_{12}N_6O.¾H_2O$

Batch Molecular Weight: 305.81

Physical Appearance: Beige solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Zhang *et al* (2021) NEK2 inhibition triggers anti-pancreatic cancer immunity by targeting PD-L1. Nat.Commun. ***12*** 4536. PMID: 34315872.

Lebraud *et al* (2014) Model system for irreversible inhibition of Nek2: thiol addition to ethynylpurines and related substituted heterocycles. Org.Biomol.Chem. ***12*** 141. PMID: 24213855.