

Certificate of Analysis

Print Date: Apr 21st 2022

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Product Name: INCB 024360-analog Catalog No.: 6007 Batch No.: 1

CAS Number: 914471-09-3

IUPAC Name: 4-Amino-N-(3-chloro-4-fluorophenyl)-N-hydroxy-1,2,5-oxadiazole-3-carboximidamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₉H₇ClFN₅O₂

Batch Molecular Weight: 271.64

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 39.8 2.6 25.77 Found 39.78 2.6 25.96



Product Information

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IUPAC Name: 4-Amino-N-(3-chloro-4-fluorophenyl)-N-hydroxy-1,2,5-oxadiazole-3-carboximidamide

Description:

INCB 024360-analog is a potent indoleamine 2,3-dioxygenase (IDO) inhibitor (IC $_{50}$ values are 19 and 67 nM in enzymatic activity and HeLa cell assays, respectively). Decreases kynurenine levels in plasma and reduces tumor growth in vivo. Cell membrane permeable.

Physical and Chemical Properties:

Batch Molecular Formula: $C_9H_7CIFN_5O_2$

Batch Molecular Weight: 271.64 Physical Appearance: Off White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

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:

Weinmann (2016) Cancer immunotherapy: selected targets and small-molecule modulators. Chem.Med.Chem. **11** 450. PMID: 26836578.

Dounay *et al* (2015) Challenges and opportunities in the discovery of new therapeutics targeting the kynurenine pathway. J.Med.Chem. *58* 8762. PMID: 26207924.

Yue *et al* (2009) Discovery of potent competitive inhibitors of indoleamine 2,3-dioxygenase with *in vivo* pharmacodynamic activity and efficacy in a mouse melanoma model. J.Med.Chem. **52** 7364. PMID: 19507862.