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TOCRIS

Print Date: Jun 15th 2023

Certificate of Analysis

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Product Name: **BAY 091** **Catalog No.: 7673** **Batch No.: 1**

CAS Number: 2922280-34-8

IUPAC Name: (*R*)-2-((3-Cyano-2-(2'-fluoro-3'-methyl-[1,1'-biphenyl]-4-yl)-1,7-naphthyridin-4-yl)amino)butanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{21}FN_4O_2$.

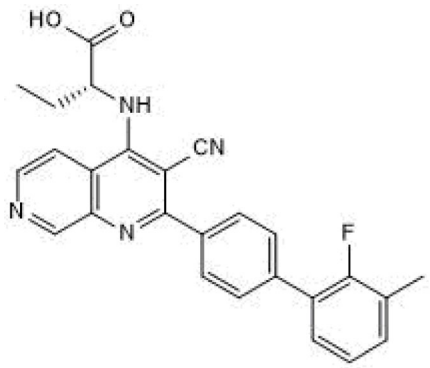
Batch Molecular Weight: 440.48

Physical Appearance: Pale yellow solid

Solubility: DMSO to 50 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

Chiral HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.9	4.81	12.72
Found	69.88	4.72	12.54

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

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Description:

BAY 091 is a potent and selective, ATP-dependent, phosphatidylinositol-5-phosphate 4-kinase type-2 alpha (PIP4K2A) inhibitor (IC_{50} values are 1.3 nM, 8.5 nM and 16.4 nM with 10 µM ATP, or in an HTRF assay with 10 µM and 2 mM ATP, respectively).

Physical and Chemical Properties:

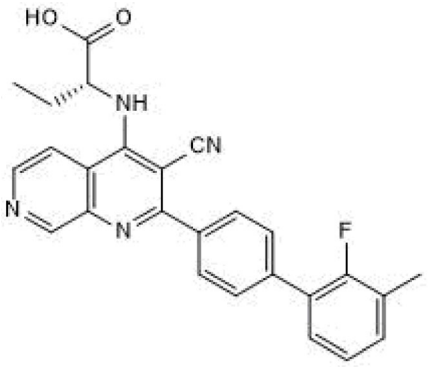
Batch Molecular Formula: $C_{26}H_{21}FN_4O_2$.

Batch Molecular Weight: 440.48

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 BAY 091 probe summary on the SGC website.

References:

Wortmann *et al* (2021) Discovery and characterization of the potent and highly selective 1,7-naphthyridine-based inhibitors BAY-091 and BAY-297 of the kinase PIP4K2A. J.Med.Chem. ***64*** 15883. PMID: 34699202.