

Product Name: Ivosidenib

Catalog No.: 7761

Batch No.: 1

CAS Number: 1448347-49-6

IUPAC Name: (2S)-N-[(1S)-1-(2-Chlorophenyl)-2-[(3,3-difluorocyclobutyl)amino]-2-oxoethyl]-1(4-cyanopyridin-2-yl)-N-(5-fluoropyridin-3-yl)-5-oxopyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₂₂ClF₃N₆O₃.

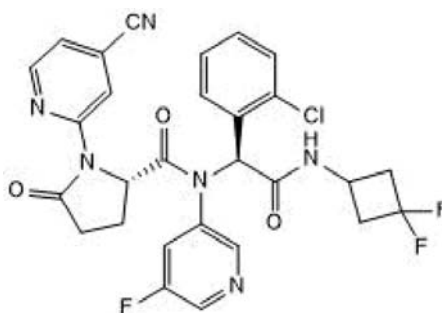
Batch Molecular Weight: 582.96

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.69	3.8	14.42
Found	57.6	3.54	14.25

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

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Description:

Ivosidenib is a potent inhibitor of mutant isocitrate dehydrogenase enzyme 1 (IDH1), with activity against a variety of mutant IDH1 enzymes (IC₅₀ range = 5-19 nM). Reduces intracellular 2-HG (Cat. No. 6122) by 96% at 0.5 μM. Increases sensitivity of melanoma to Temozolomide (Cat. No. 2706) in vivo and inhibits wild-type IDH1 in low magnesium and low nutrient levels. Ivosidenib also inhibits growth of tumors in cell and animal models of pancreatic cancer and inhibits invasion and migration of chondrosarcoma cells in vitro. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

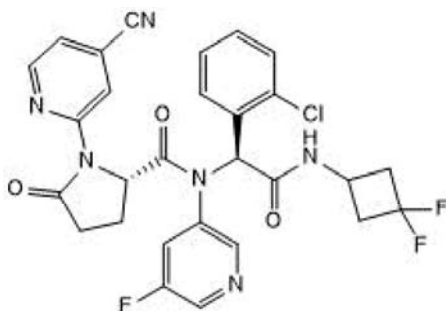
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Batch Molecular Weight: 582.96

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Zarei *et al* (2022) Wild-type IDH1 inhibition enhances chemotherapy response in melanoma. *J.Exp.Clin.Cancer Res.* **41** 283. PMID: 36153582.

Popovici-Muller *et al* (2018) Discovery of AG-120 (ivosidenib): a first-in-class mutant IDH1 inhibitor for the treatment of IDH1 mutant cancers. *ACS Med.Chem.Lett.* **9** 300. PMID: 29670690.

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.

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