

Product Name: TC-S 7005

Catalog No.: 4459

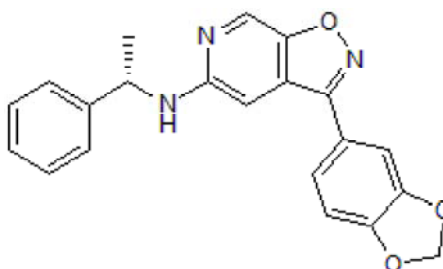
Batch No.: 3

CAS Number: 1082739-92-1

IUPAC Name: 3-(1,3-Benzodioxol-5-yl)-N-[(1S)-1-phenylethyl]-isoxazolo[5,4-c]pyridin-5-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₁₇N₃O₃
Batch Molecular Weight: 359.38
Physical Appearance: Cream solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:Petroleum ether [1:4])
HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -63.1 (Concentration = 1, Solvent = Chloroform)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.18	4.77	11.69
Found	69.9	4.87	11.66

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

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Description:

Potent and selective polo-like kinase 2 (PLK2) inhibitor (IC_{50} = 4 nM). Shows selectivity for PLK2 over PLK3 and PLK1 (IC_{50} values are 24 and 214 nM respectively). Induces mitotic arrest and cell death in HCT 116 colorectal cells.

Physical and Chemical Properties:

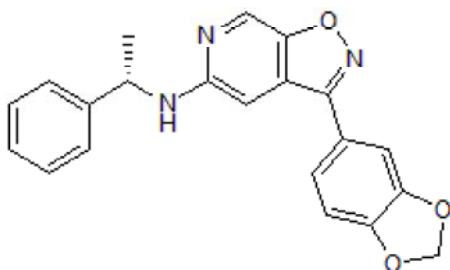
Batch Molecular Formula: $C_{21}H_{17}N_3O_3$

Batch Molecular Weight: 359.38

Physical Appearance: Cream solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO 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:

Hanan *et al* (2008) Design and synthesis of 2-amino-isoxazolopyridines as Polo-like kinase inhibitors. *Bioorg.Med.Chem.Lett.* **18** 5186. PMID: 18790636.

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