

Product Name: CHDI 00580985

Catalog No.: 7881

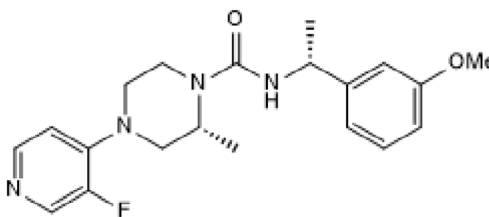
Batch No.: 1

CAS Number: 2573071-18-6

IUPAC Name: (2*R*)-4-(3-Fluoro-4-pyridinyl)-*N*-[(1*R*)-1-(3-methoxyphenyl)ethyl]-2-methyl-1-piperazinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₅FN₄O₂.
Batch Molecular Weight: 372.44
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 98.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.5	6.77	15.04
Found	63.8	6.78	15.03

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

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Description:

CHDI 00580985 is a potent and selective ROCK inhibitor (IC₅₀ values are 3 nM and 8 nM in biochemical (ROCK2) and cellular assays respectively). CHDI 00580985 inhibits ROCK-mediated substrate (MYPT1) phosphorylation (IC₅₀ = 4 nM). In vivo, CHDI 00580985 reduces ROCK signaling in Huntington's disease mouse models in pharmacodynamic assay. CHDI 00580985 is bioavailable and brain penetrant.

Physical and Chemical Properties:

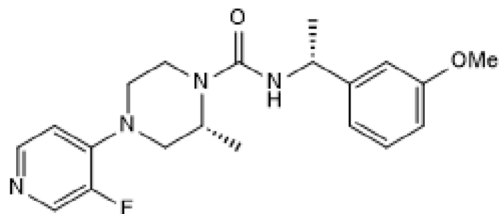
Batch Molecular Formula: C₂₀H₂₅FN₄O₂.

Batch Molecular Weight: 372.44

Physical Appearance: White solid

Minimum Purity: ≥98%

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. *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:

Sold under license from CHDI Foundation

References:

Ladduwahetty *et al* (2022) Identification of a potent, selective, and brain-penetrant Rho kinase inhibitor and its activity in a mouse model of Huntington's disease. *J.Med.Chem.* **65** 9819. PMID: 35816678.

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