

Product Name: CHDI 00484077

Catalog No.: 7879

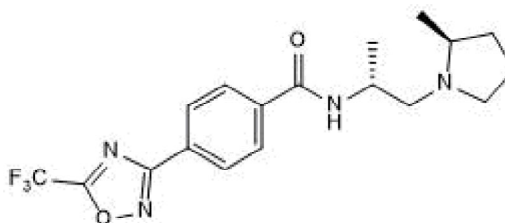
Batch No.: 1

CAS Number: 3025894-92-9

IUPAC Name: *N*-((*R*)-1-((*S*)-2-Methylpyrrolidin-1-yl)propan-2-yl)-4-(5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₁F₃N₄O₂
Batch Molecular Weight: 382.39
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM with gentle warming
 ethanol to 100 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.54	5.54	14.65
Found	56.58	5.48	14.55

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

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Description:

CHDI 00484077 is a potent and selective class IIa histone deacetylase HDAC inhibitor (IC₅₀ values = 10-30 nM in vivo, 0.01 nM and 0.04 nM in HEK293 and Jurkat cells, respectively). Exhibits 150-fold selectivity for class IIa over class I/IIb HDACs in cells. Orally bioavailable and CNS penetrant.

Physical and Chemical Properties:

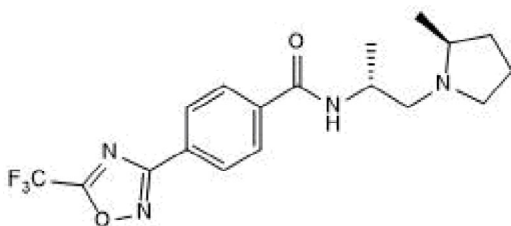
Batch Molecular Formula: C₁₈H₂₁F₃N₄O₂

Batch Molecular Weight: 382.39

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM with gentle warming
ethanol to 100 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:

Sold under license from CHDI Foundation

References:

Stott et al (2021) Evaluation of 5-(trifluoromethyl)-1,2,4-oxadiazole-based class IIa HDAC inhibitors for Huntington's disease. ACS Med.Chem.Lett **12** 380. PMID: 33738065.

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