

Product Name: NVS MLLT-1

Catalog No.: 7482

Batch No.: 1

CAS Number: 2561471-13-2

IUPAC Name: *N*-[2-[[*(2S)*-2-Methyl-1-pyrrolidinyl]methyl]-1*H*-benzimidazol-6-yl]-6-isoquinolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₃N₅O.¼H₂O

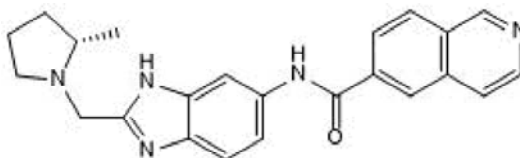
Batch Molecular Weight: 389.97

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.84	6.07	17.96
Found	71.04	6.02	18.03

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

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Description:

NVS-MLLT-1 is a selective inhibitor of YEATS domain of MLLT1 and MLLT3 (IC₅₀ values are 150 and 254 nM for MLLT1 and MLLT3, respectively). It shows selectivity for YEATS2/4 domains and over all bromodomains (CERC2 IC₅₀ > 40 μM).

Physical and Chemical Properties:

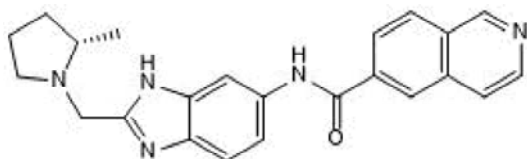
Batch Molecular Formula: C₂₃H₂₃N₅O.¼H₂O

Batch Molecular Weight: 389.97

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the NVS MLLT-1 probe summary on the SGC website.

References:

Ni *et al* (2021) Structure and inhibitor binding characterization of oncogenic MLLT1 mutants. ACS Chem.Biol. **16** 571. PMID: 33749253.

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