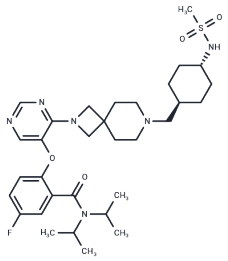
# Data Sheet (Cat.No.T13336)

TargetMol

VTP50469

## Chemical Properties



CAS No. : 2169916-18-9

Formula: C32H47FN6O4S

Molecular Weight: 630.82

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

## Biological Description

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|---|---|
| Description | VTP50469 is a highly selective and orally active small molecule inhibitor of the Menin-MLL protein-protein interaction with potent anti-leukemic activity with a Ki of 104 pM. |
| Targets(IC50) | Apoptosis,Epigenetic Reader Domain,Histone Methyltransferase |
| In vitro | VTP50469 inhibits cell proliferation in a concentration-dependent manner in MLL-r cell lines, including (MOLM13 with IC50 of 13 nM), THP1 (IC50 of 37 nM), NOMO1 (IC50 of 30 nM), ML2 (IC50 of 16 nM), EOL1 (IC50 of 20 nM), and murine MLL-AF9 cells (IC50 of 15 nM)), as well as ALL cell lines (KOPN8 (IC50 of 15 nM), HB11;19 (IC50 of 36 nM), MV4;11 (IC50 of 17 nM), SEMK2 (IC50 of 27 nM), and RS4;11 (IC50 of 25 nM)). At early timepoints, MLL-r B cell ALL (B-ALL) cell lines, but not MLL-r AML cell lines, underwent dose-dependent apoptosis in response to VTP50469, while MLL-r AML cell lines exhibited dose-dependent differentiation starting at 4-6 days of exposure. VTP50469 displaces Menin from protein complexes, reducing MLL chromatin occupancy on certain genes, resulting in altered gene expression, differentiation, and apoptosis [1]. |
| In vivo | **METHODS**: MV4-transplanted NSG mice were treated with VTP50469 (15, 30, and 60 mg/kg, orally twice a day) and the tumor growth in vivo was observed.<br>**RESULTS** The size of subcutaneous tumors in mice decreased in a dose-dependent manner. [1] |

## Solubility Information

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|---|---|
| Solubility | DMSO: 125 mg/mL (198.15 mM),Sonication is recommended.<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |
| In vivo Formulation | 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (6.34 mM),Sonication is recommended.<br>*Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.* |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 1 mM | 1.5852 mL | 7.9262 mL | 15.8524 mL |
| 5 mM | 0.317 mL | 1.5852 mL | 3.1705 mL |
| 10 mM | 0.1585 mL | 0.7926 mL | 1.5852 mL |
| 50 mM | 0.0317 mL | 0.1585 mL | 0.317 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Krivtsov AV, et al. A Menin-MLL Inhibitor Induces Specific Chromatin Changes and Eradicates Disease in Models of MLL-Rearranged Leukemia. Cancer Cell. 2019 Dec 9;36(6):660-673.
Andrei V. Krivtsov, et al. Abstract 4958: VTP50469 is a novel, orally available menin-MLL1 inhibitor effective against MLL-rearranged and NPM1-mutant leukemia. Cancer Resceach. July 2018.Volume 78, Issue 13 Supplement.