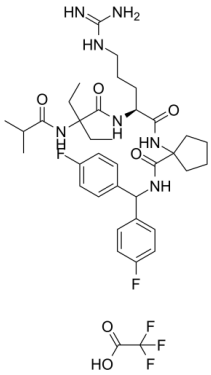
Data Sheet

Product Name:	MM-102 (TFA)
Cat. No.:	CS-5186
CAS No.:	1883545-52-5
Molecular Formula:	C37H50F5N7O6
Molecular Weight:	783.83
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : ≥ 100 mg/mL (127.58 mM)



BIOLOGICAL ACTIVITY:

MM-102 TFA (HMTase Inhibitor IX TFA) is a potent WDR5/MLL interaction inhibitor, achieves IC50 = 2.4 nM with an estimated Ki < 1 nM in WDR5 binding assay, which is >200 times more potent than the ARA peptide. IC50 & Target: IC50: 2.4 nM (MLL)[1]. **In Vitro:** MM-102 (HMTase Inhibitor IX) inhibits MLL1 methyltransferase activity and MLL-1-induced HoxA9 and Meis-1 gene expression in leukemia cells expressing the MLL1-AF9 fusion gene. Also inhibits cell growth and induces apoptosis in leukemia cells harbouring MLL1 fusion proteins.

MM-102 (TFA), with the highest binding affinities to WDR5, also show the most potent inhibitory activity in the HMT assay withIC_{50} =0.4-0.9 μM[1].

MM-102 (HMTase Inhibitor IX) dose-dependently inhibits cell growth in the MV4;11 and KOPN8 leukemia cell lines, which carry MLL1-AF4 and MLL1-ENL fusion proteins, respectively[1].

MM-102 (HMTase Inhibitor IX) has IC_{50}=25 μM in both cell lines and completely inhibits cell growth in these cell lines at 75 μM[1].

MM-102 (HMTase Inhibitor IX) effectively and selectively inhibits cell growth and induces apoptosis in leukemia cells harboring MLL1 fusion proteins and has minimal effect in leukemia cells with wild-type MLL1 protein[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: MV4;11, KOPN8, and K562 cells were cultured in RPMI 1640 medium (ATCC) supplemented with 10% fetal bovine serum and 100 U/L penicillinstreptomycin and incubated at 37°C under 5% CO2. Cells were seeded into 12-well plates for suspension at a density of 5 × 105 per well (1 mL) and treated with either vehicle control (DMSO, 0.2%) or MM-102 (HMTase Inhibitor IX) for 7 days. The medium was changed every 2 days, and compounds were resupplied. The CellTiter-Glo Luminescent Cell Viability Assay kit was used. First, 100 μL of the assay reagent was added into each well, and the content was mixed for 2 min on an orbital shaker to induce cell lysis. After 10 min incubation at room temperature, the luminescence was read on a microplate reader.

References:

[1]. Karatas H, et al. High-affinity, small-molecule peptidomimetic inhibitors of MLL1/WDR5 protein-protein interaction. J Am Chem Soc. 2013 Jan 16;135(2):669-682.

CAIndexNames:

(S)-N-(bis(4-fluorophenyl)methyl)-1-(2-(2-ethyl-2-isobutyramidobutanamido)-5-guanidinopentanamido)cyclopentanecarboxamide 2,2,2-trifluoroacetate

SMILES:

O=C(C1(NC([C@@H](NC(C(NC(C(C)C)=O)(CC)CC)=O)CCCNC(N)=N)=O)CCCC1)NC(C2=CC=C(F)C=C2)C3=CC=C(F)C=C3.FC(F)(F)C(O)=O

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA