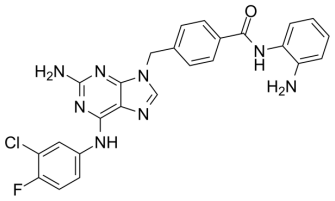
HDAC-IN-45

Cat. No.:	HY-150577
CAS No.:	2421122-61-2
Molecular Formula:	$C_{25}H_{20}ClFN_8O$
Molecular Weight:	502.93
Target:	HDAC
Pathway:	Cell Cycle/DNA Damage; Epigenetics
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

HDAC-IN-45 (Compound 14) is a small molecule HDAC inhibitor and has anticancer activity, also can forms a hydrogenbond with residue Y303. HDAC-IN-45 (Compound 14) has substantial inhibitory effects towards HDAC1, 2 and 3 isoforms with IC_{50} values of 0.108, 0.585 and 0.563 μM respectively[1].

IC_{50} & Target

HDAC1	HDAC2	HDAC3	HDAC6
0.108 μM (IC_{50})	0.585 μM (IC_{50})	0.563 μM μM (IC_{50})	⊠10 μM (IC_{50})

HDAC8
6.81 μM (IC_{50})

In Vitro

HDAC-IN-45 (Compound 14) suppresses the growth of triple-negative breast cancer cells MDA-MB-231 (IC_{50} = 1.48 μM), MDA-MB-468 (IC_{50}= 0.65 μM), and liver cancer cells HepG2 (IC_{50}= 2.44 μM).
HDAC-IN-45 has equally virulent in the HDAC-sensitive cell lines (YCC11) and -resistant gastric cell lines (YCC3/7) and overcome HDACi resistance. HDAC-IN-45 has a high toxicity (IC_{50}= 0.33 μM) in three leukemic cell lines, K-562, KG-1 and THP-1.
HDAC-IN-45 (Compound 14) has substantial inhibitory effects towards HDAC1, 2 and 3 isoforms with IC_{50} values of 0.108, 0.585 and 0.563 μM respectively.
HDAC-IN-45 (Compound 14) can elevate acetylation level of histone H3 and expression of p21.
HDAC-IN-45 (Compound 14) exerts a dose-dependent upregulation of ac-H3K9 in MDA-MB-231 cells, triggers cell cycle arrest in G1 phase.
HDAC-IN-45 (Compound 14) exhibits a potent antitumor efficacy in xenograft mouse model[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	Triple-negative breast cancer cells; liver cancer cells; YCC11 and YCC3/7
Concentration:	a series of concentration
Incubation Time:	72 h
Result:	Inhibited the cell growth viability of HepG2 and triple-negative breast cancer cells.

Cell Cytotoxicity Assay[1]

Cell Line:	Three leukemic cell lines (K-562, KG-1 and THP-1); YCC3/7 and YCC11 cell lines
Concentration:	a series of concentration
Incubation Time:	72 h
Result:	Showed a potent anti-cancer effect, exhibited high sensitivities and strong toxicities with IC50 values below micromolar in leukemic cell lines.

Western Blot Analysis[1]

Cell Line:	MDA-MB-231 cells
Concentration:	2 μM
Incubation Time:	24 h
Result:	Elevated acetylation level of histone H3 and expression of p21.

Cell Cycle Analysis[1]

Cell Line:	MDA-MB-231cells
Concentration:	4 μM
Incubation Time:	24 h
Result:	Arrested cell cycle in G1 and trigger apoptosis.

In Vivo

HDAC-IN-45 (Compound 14) (25 mg/kg or 50mg/kg; i.p.; every day) exhibits a potent antitumor efficacy in human MDA-MB-231 breast cancer xenograft mouse model[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Human MDA-MB-231 breast cancer xenograft mouse model[1]
Dosage:	25 mg/kg or 50mg/kg
Administration:	25 mg/kg or 50mg/kg; i.p.; every day.
Result:	Exhibited a potent antitumor efficacy.

REFERENCES

[1]. Kunal Nepali, et al. Purine/purine isoster based scaffolds as new derivatives of benzamide class of HDAC inhibitors. Eur J Med Chem. 2020 Jun 15;196:112291.

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