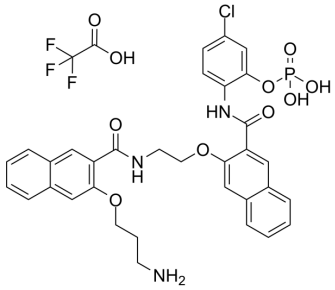
CREB-IN-1 TFA

Cat. No.:	HY-144318
CAS No.:	2912285-84-6
Molecular Formula:	$C_{35}H_{32}ClF_3N_3O_{10}P$
Molecular Weight:	778.06
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	CREB-IN-1 TFA is a potent, orally active CREB inhibitor (IC_{50}=0.18 μM). CREB-IN-1 TFA inhibits breast cancer cell growth[1].
IC_{50} & Target	IC_{50}: 0.18 μM (CREB)[1]

In Vitro

CREB-IN-1 TFA (compound 3) (HEK 293T cells; 100 μM; 24 hours) inhibits CREB-mediated gene transcription with an IC_{50} of 0.18 μM[1].

CREB-IN-1 TFA (100 μM; 3 days) shows potent activities in MDA-MB-231 (GI_{50}=0.38 μM) and MDA-MB-468 (GI_{50}=0.021 μM) cells [1].

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

Cell Viability Assay[1]

Cell Line:	HEK 293T cells
Concentration:	100 μM
Incubation Time:	24 hours
Result:	Inhibited CREB-mediated gene transcription with an IC_{50} of 0.18 μM.

Cell Proliferation Assay[1]

Cell Line:	MDA-MB-231, MDA-MB-468 cells
Concentration:	100 μM
Incubation Time:	3 days
Result:	Showed potent activities in MDA-MB-231 (GI_{50} =0.38 μM) and MDA-MB-468 (GI_{50} =0.021 μM) cells.

In Vivo

CREB-IN-1 TFA (5, 10, 20 mg/kg) shows much improve oral bioavailability at 38%[1].

Pharmacokinetic Parameters of CXCR4 antagonist 4 in mice [1].

route	dose(mg/kg)	$t_{1/2}$(h)	T_{max}(h)	C_{max}(ng/mL)	AUC_{0-t} (ng·hr/mL)	$AUC_{0-\infty}$ ((ng·hr/mL)	bioavailability (F%)
IP	10	4.2	1.0	156	892	910	144
PO	20	5.5	2.00	73	468	479	38

Mice, 5 mg/kg IV; 10 mg/kg IP; 20 mg/kg PO[1].

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

Animal Model:	Female C57BL/6 mice[1]
Dosage:	5, 10, 20 mg/kg (dissolved in 0.1 N NaOH in ddI H_2O at 40 mg/mL and further dilutions were made using ddI H_2O)
Administration:	Showed much improve oral bioavailability at 38%.
Result:	Showed much improve oral bioavailability at 38%.

REFERENCES

[1]. Peng J, et al. Design, Synthesis and Biological Evaluation of Prodrugs of 666-15 as Inhibitors of CREB-Mediated Gene Transcription. ACS Med Chem Lett. 2022; 13(3):388-395.

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