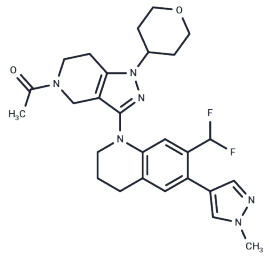
Data Sheet (Cat.No.T15397)

TargetMol

GNE-049

Chemical Properties



CAS No. : 1936421-41-8

Formula: C27H32F2N6O2

Molecular Weight: 510.58

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

Description	GNE-049 is a highly selective and potent inhibitor designed to target the CREB-binding protein (CBP) with high affinity, exhibiting an IC50 of 1.1 nM for the suppression of BRET and BRD4 activity, which consequently blocks prostate cancer cell proliferation in both in vitro and in vivo models.
Targets(IC50)	Epigenetic Reader Domain,Histone Acetyltransferase
In vitro	GNE-049 performs well in BRET cell assays and, in an orthogonal targeted assay, inhibits MYC expression (MV4-11 cell line) with an EC50 of 14 nM.[1] CBPD-409 induced strong degradation of CBP/p300 by DC 500.2-0.4 nM and exhibited strong antiproliferative effects with IC50 of 1.2-2.0 nM in VCaP, LNCaP, and 22Rv1 AR+ prostate cancer cell lines. [2]
In vivo	GNE-049 shows acceptable PK in mouse, rat, dog, and monkey. GNE-049 is further evaluated in a rat single dose (30-250 mg/kg QD) toxicokinetic study. GNE-049 is selective for CBP/P300 and, importantly, quite selective (3820-fold) over BRD4(1), which revealed from the Determination of potency versus a selection of bromodomains. Furthermore, at the 250 mg/kg dose level, the ratio of the unbound drug concentration in the brain to unbound drug concentration in plasma (Kp,uu) 3 h post-dose is determined to be 0.43, indicating that GNE-049 is penetrating into the CNS and potentially resulting in the observed toxicity.

Solubility Information

Solubility	DMSO: 80 mg/mL (156.68 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (6.46 mM),Sonication is recommended. *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	1.9586 mL	9.7928 mL	19.5856 mL
5 mM	0.3917 mL	1.9586 mL	3.9171 mL
10 mM	0.1959 mL	0.9793 mL	1.9586 mL
50 mM	0.0392 mL	0.1959 mL	0.3917 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

Romero FA, et al. GNE-781, A Highly Advanced Potent and Selective Bromodomain Inhibitor of Cyclic Adenosine Monophosphate Response Element Binding Protein, Binding Protein (CBP). J Med Chem. 2017 Nov 22;60(22):9162-9183.

Nguyen D T, Mahajan U, Angappulige D H, et al.Amino Terminal Acetylation of HOXB13 Regulates the DNA Damage Response in Prostate Cancer.Cancers.2024, 16(9): 1622.

Fiskus W, et al. Preclinical efficacy of CDK7 inhibitor-based combinations against myeloproliferative neoplasms transformed to AML. Blood. 2025 Feb 6;145(6):612-624.

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481