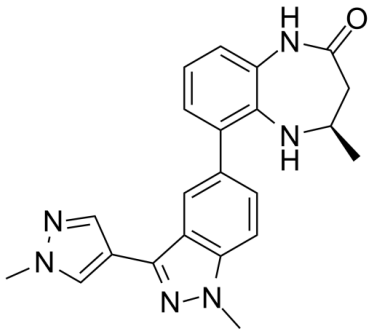
Data Sheet

Product Name:	CPI-637
Cat. No.:	CS-5946
CAS No.:	1884712-47-3
Molecular Formula:	$C_{22}H_{22}N_6O$
Molecular Weight:	386.45
Target:	Epigenetic Reader Domain; Histone Acetyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : 9.62 mg/mL (24.89 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

CPI-637 is a selective and potent **CBP/EP300** bromodomain inhibitor with **IC_{50}** values of 0.03 μM, 0.051 μM and 11.0 μM for **CBP**, **EP300** and **BRD4 BD-1**, respectively, and an **EC_{50}** of 0.3 μM for **CBP**[1]. **In Vitro:** CPI-637 (Compound 28) inhibits MYC expression in AMO-1 cells (**EC_{50}** value of 0.60 μM) [1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase assay: CPI-637 potencies were evaluated in a panel of biochemical bromodomain binding assays. Binding of biotinylated small molecule ligand or biotinylated histone H3K14 peptide ligand (BAZ2B) to recombinant His-tagged bromodomains was assessed by time-resolved fluorescence resonance energy transfer (TR-FRET). Test compounds that compete with the biotinylated ligand for bromodomain binding reduce the TR-FRET signal. Assays were conducted in a total volume of 15 μL in white 384-well plates with the DMSO oncentration held constant at 0.2%. All reagents were prepared in assay buffer (50 mM HEPES pH 7.5, 1 mM TCEP, 0.069 mM Brij-35, 50 mM NaCl, and 0.1 mg/mL bovine serum albumin). Compounds in DMSO were added to empty assay plates using an Echo 550 acoustic dispenser . Bromodomain was added followed by biotinylated ligand, and the plates were incubated for 10 minutes after each addition (20 minutes for BAZ2B). Subsequently, the TR-FRET detection reagents, anti-Hiseuropium and streptavidin-allophycocyanin were added and incubated for an additional 40 minutes. Compounds were evaluated as 10-point titrations with N = 2. Each compound was assayed in at least 3 independent assays. Results were analyzed with XLFit beginning with a 4-parameter Hill fit and constraining one or more parameters if necessary to generate a suitable fit. [1]

References:

[1]. Taylor AM, et al. Fragment-Based Discovery of a Selective and Cell-Active Benzodiazepinone CBP/EP300 Bromodomain Inhibitor (CPI-637). ACS Med Chem Lett. 2016 Mar 15;7(5):531-6.

CAIndexNames:

2H-1,5-Benzodiazepin-2-one, 1,3,4,5-tetrahydro-4-methyl-6-[1-methyl-3-(1-methyl-1H-pyrazol-4-yl)-1H-indazol-5-yl]-, (4R)-

SMILES:

O=C1NC2=CC=CC(C3=CC4=C(N(C)N=C4C5=CN(C)N=C5)C=C3)=C2N[C@H](C)C1

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

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