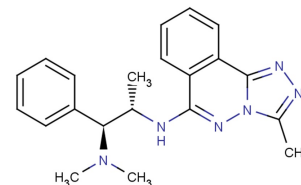


L-45

**Chemical Properties**

CAS No.:	2079885-05-3
Formula:	C <sub>21</sub> H <sub>24</sub> N <sub>6</sub>
Molecular Weight:	360.46
Appearance:	N/A
Storage:	0-4°C for short term (days to weeks), or -20°C for long term (months).

**Biological Description**

Description	L-45 is the first potent and cell-active bromodomain (Brd) inhibitor of p300/CBP-associated factor (PCAF) (K <sub>d</sub> : 126±15 nM).
Targets(IC <sub>50</sub> )	Brd: 126 nM (kd)
In vitro	L-45 binds in the acetylated lysines (KAc) -binding pocket of PfGCN (blue ribbon and sticks) and makes H-bonds (dotted lines) through the triazole to N1436 and the first of a network of four water molecules (red spheres). A structure using highly homologous (64 % identity) Brd from Plasmodium falciparum, PfGCN5, of which L-45 is also a potent ligand (isothermal titration calorimetry (ITC) K <sub>D</sub> 280 nM), is successfully obtained (PDB: 5TPX). L-45 disrupts PCAF-Brd histone H3.3 interaction in cells using a nanoBRET assay, and a co-crystal structure of L-45 with the homologous Brd PfGCN5 from Plasmodium falciparum rationalizes the high selectivity for PCAF and GCN5 bromodomains.
In vivo	In human and mouse liver microsomes, L-45 displays no observable cytotoxicity in peripheral blood mononuclear cells (PBMC), good cell-permeability, and metabolic stability. It also supports its potential for in vivo use.

**Solubility Information**

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble
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## Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.774 mL	13.871 mL	27.742 mL
5 mM	0.555 mL	2.774 mL	5.548 mL
10 mM	0.277 mL	1.387 mL	2.774 mL
50 mM	0.055 mL	0.277 mL	0.555 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 °C for 6 months; - 20 °C for 1 month. Please use it as soon as possible.

## Reference

1. Moustakim M, et al. Discovery of a PCAF Bromodomain Chemical Probe. Angew Chem Int Ed Engl. 2017 Jan 16;56(3):827-831.

Inhibitors · Natural Compounds · Compound Libraries

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