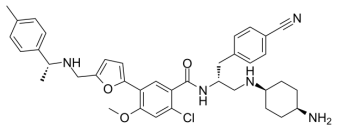
BAY-850

Cat. No.:	HY-119254
CAS No.:	2099142-76-2
Molecular Formula:	$C_{38}H_{44}ClN_5O_3$
Molecular Weight:	654.24
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 62.5 mg/mL (95.53 mM; Need ultrasonic)

H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.5285 mL	7.6425 mL	15.2849 mL
5 mM	0.3057 mL	1.5285 mL	3.0570 mL
10 mM	0.1528 mL	0.7642 mL	1.5285 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 6.25 mg/mL (9.55 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 6.25 mg/mL (9.55 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-850 is a potent and isoform selective ATPase family AAA domain-containing protein 2 (ATAD2) inhibitor, with an IC_{50} of 166 nM.

IC_{50} & Target

ATAD2[1].

In Vitro

BAY-850 competes with the binding of a mono-acetylated Histone H4 N-terminal peptide to ATAD2 BD with an IC_{50} of 166 nM measured in TR-FRET assay. BAY-850 displaces the tetra-acetylated peptide with an IC_{50} of 157 nM and a K_D of 115 nM respectively. The unprecedented isoform selectivity of BAY-850 suggests a different mode of action to those exhibited by canonical BD inhibitors[1].

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

CUSTOMER VALIDATION

- Commun Biol. 2021 Mar 25;4(1):399.
- J Enzyme Inhib Med Chem. 2023 Dec;38(1):2242601.
- Eur Rev Med Pharmaco. 2020 Oct;24(19):9860-9868.
- Discov Oncol. 2023 May 26;14(1):79.

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REFERENCES

[1]. Fernández-Montalván AE, et al. Isoform-Selective ATAD2 Chemical Probe with Novel Chemical Structure and Unusual Mode of Action. ACS Chem Biol. 2017 Nov 17;12(11):2730-2736.

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