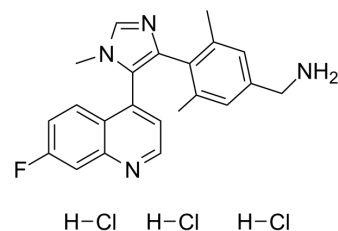


BI-9321 trihydrochloride

Cat. No.:	HY-114208A
CAS No.:	2387510-87-2
Molecular Formula:	C ₂₂ H ₂₄ Cl ₃ FN ₄
Molecular Weight:	469.81
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Storage:	4°C, stored under nitrogen, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (532.13 mM; Need ultrasonic)
H₂O : 25 mg/mL (53.21 mM; Need ultrasonic)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	2.1285 mL	10.6426 mL	21.2852 mL
	5 mM	0.4257 mL	2.1285 mL	4.2570 mL
	10 mM	0.2129 mL	1.0643 mL	2.1285 mL

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

In Vivo

- Add each solvent one by one: PBS
Solubility: 100 mg/mL (212.85 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 25 mg/mL (53.21 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 25 mg/mL (53.21 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 25 mg/mL (53.21 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BI-9321 trihydrochloride is a potent, selective and cellular active nuclear receptor-binding SET domain 3 (NSD3)-PWWP1 domain antagonist with a K_d value of 166 nM. BI-9321 trihydrochloride is inactive against NSD2-PWWP1 and NSD3-PWWP2. BI-9321 trihydrochloride specifically disrupts histone interactions of the NSD3-PWWP1 domain with an IC₅₀ of 1.2 μM in U2OS cells^[1].

IC₅₀ & Target	Kd: 166 nM (NSD3-PWWP1) ^[1]
In Vitro	BI-9321 trihydrochloride is targeting the methyl-lysine binding site of the PWWP1 domain with sub-micromolar in vitro activity and cellular target engagement at 1 μM. As a single agent, BI-9321 trihydrochloride downregulates Myc messenger RNA expression and reduces proliferation in MOLM-13 cells ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Böttcher J, et al. Fragment-based discovery of a chemical probe for the PWWP1 domain of NSD3. Nat Chem Biol. 2019 Aug;15(8):822-829.

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

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