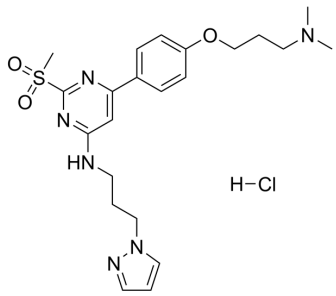
TP-238 hydrochloride

Cat. No.:	HY-114205A
CAS No.:	2415263-05-5
Molecular Formula:	$C_{22}H_{31}ClN_6O_3S$
Molecular Weight:	495.04
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	-20°C, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (202.00 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.0200 mL	10.1002 mL	20.2004 mL
5 mM	0.4040 mL	2.0200 mL	4.0401 mL
10 mM	0.2020 mL	1.0100 mL	2.0200 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: ≥ 2.5 mg/mL (5.05 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.05 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.05 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TP-238 hydrochloride is a potent and selective dual CECR2/BPTF probe with IC_{50} values of 30 nM and 350 nM, respectively. TP-238 hydrochloride also inhibits BRD9 with a pIC_{50} of 5.9 and is less active against other 338 kinases[1][2].

IC_{50} & Target

CECR2 30 nM (IC_{50})	CECR2 10 nM (Kd)	CECR2 7.5 (pIC_{50})	BPTF 350 nM (IC_{50})
BPTF 120 nM (Kd)	BPTF 6.5 (pIC_{50})	BRD9 5.9 (pIC_{50})	

In Vitro	TP-238 has on target biochemical activity of 10-30 nM with CECR2 and 100-350 nM with BPTF. TP-238 displays potency for both CECR2 (pIC50 of 7.5) and BPTF (pIC50 of 6.5) in an Alpha screen assay. Isothermal titration calorimetry (ITC) shows TP-238 with a Kd of 10 nM for CECR2 and 120 nM for BPTF[1][2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Michael A Clegg, et al. Advancements in the Development of non-BET Bromodomain Chemical Probes. ChemMedChem. 2019 Feb 19;14(4):362-385.

[2]. Peter D Ycas, et al. New Inhibitors for the BPTF Bromodomain Enabled by Structural Biology and Biophysical Assay Development. Org Biomol Chem. 2020 Jun 26.

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