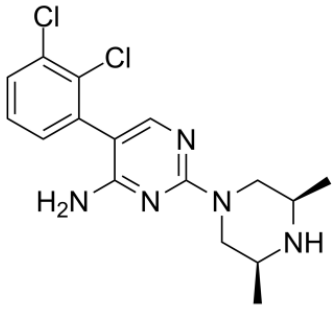
SHP836

Cat. No.:	HY-121879
CAS No.:	1957276-35-5
Molecular Formula:	$C_{16}H_{19}Cl_2N_5$
Molecular Weight:	352.26
Target:	Phosphatase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (**709.70 mM;** Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8388 mL	14.1941 mL	28.3881 mL
	5 mM	0.5678 mL	2.8388 mL	5.6776 mL
	10 mM	0.2839 mL	1.4194 mL	2.8388 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 (17.74 mM); Clear solution
2. Add each solvent one by one: **10% DMSO >> 90% (20% SBE-β-CD in saline)**
   Solubility: ≥ 6.25 mg/mL (17.74 mM); Clear solution
3. Add each solvent one by one: **10% DMSO >> 90% corn oil**
   Solubility: ≥ 6.25 mg/mL (17.74 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	SHP836 is a **SHP2** allosteric inhibitor, with an **IC_{50}** of 12 μM for the full length SHP2[1].
IC_{50} & Target	IC50: 12 μM (SHP2)[1]
In Vitro	SHP836 stabilizes the active conformation of SHP2, in which the catalytic site is blocked and no longer accessible to substrate[1].

REFERENCES

[1]. Liu WS, et al. Structure based design of selective SHP2 inhibitors by De novo design, synthesis and biological evaluation. J Comput Aided Mol Des. 2019 Aug;33(8):759-774.

[2]. Garcia Fortanet J, et al. Allosteric Inhibition of SHP2: Identification of a Potent, Selective, and Orally Efficacious Phosphatase Inhibitor. J Med Chem. 2016 Sep 8;59(17):7773-82.

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