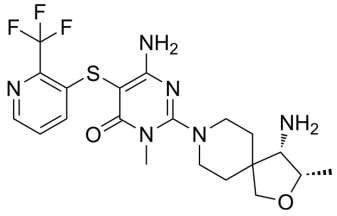
SHP394

Cat. No.:	HY-114397
CAS No.:	2055757-40-7
Molecular Formula:	$C_{20}H_{25}F_3N_6O_2S$
Molecular Weight:	470.51
Target:	Phosphatase; SHP2
Pathway:	Metabolic Enzyme/Protease; Protein Tyrosine Kinase/RTK
Storage:	4°C, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 24 mg/mL (51.01 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1254 mL	10.6268 mL	21.2535 mL
	5 mM	0.4251 mL	2.1254 mL	4.2507 mL
	10 mM	0.2125 mL	1.0627 mL	2.1254 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 (13.28 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 6.25 mg/mL (13.28 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 6.25 mg/mL (13.28 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SHP394 is an orally active, selective and allosteric inhibitor of SHP2, with an IC_{50} of 23 nM[1].

IC_{50} & Target

IC50: 23 nM (SHP2)[1]

In Vitro

SHP394 inhibits Caco-2 cells proliferation with the IC_{50} of 297 nM[1].
SHP394 exhibits antiproliferation activity against the Detroit-562 pharyngeal carcinoma cell line in vitro (IC_{50}= 1.38 μM) [1].
SHP394 decreases p-ERK with an IC_{50} of 18 nM KYSE520 cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

SHP394 (20-80 mg/kg; oral gavage; twice daily) dose-dependent reduces tumor volume[1].
SHP394 (80 mg/kg; oral gavage; twice daily) causes tumor 34% regression and reduces mouse host bodyweight after dosing for 14 days[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Six-week old female athymic NU/NU mice were inoculated subcutaneously with Detroit-562 pharyngeal carcinoma cells[1].
Dosage:	20, 40, and 80 mg/kg
Administration:	Oral gavage; twice daily
Result:	Demonstrated a clear dose-dependent reduction in tumor volume.

REFERENCES

[1]. Sarver P, et al. 6-Amino-3-methylpyrimidinones as Potent, Selective, and Orally Efficacious SHP2 Inhibitors. J Med Chem. 2019 Feb 28;62(4):1793-1802.

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