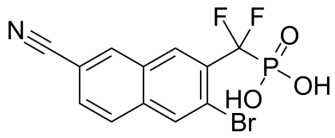
PTP1B-IN-3

Cat. No.:	HY-15133
CAS No.:	809272-64-8
Molecular Formula:	$C_{12}H_7BrF_2NO_3P$
Molecular Weight:	362.06
Target:	Phosphatase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (138.10 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7620 mL	13.8099 mL	27.6197 mL
	5 mM	0.5524 mL	2.7620 mL	5.5239 mL
	10 mM	0.2762 mL	1.3810 mL	2.7620 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 (6.90 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.90 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.90 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PTP1B-IN-3 is a potent and orally active PTP1B inhibitor with IC_{50}s of 120 nM for both PTP1B and TCPTP. PTP1B-IN-3 has antidiabetic and anticancer effects[1][2].

IC_{50} & Target

IC50: 120 nM (PTP1B), 120 nM (TCPTP) [2]

In Vivo

In diet-induced obese (DIO) mice, PTP1B-IN-3 (compounds 3g) exhibits dose dependent inhibition (60%, 80% and 100% inhibition at 1, 3 and 10 mg/kg, respectively) of glucose excursion when given orally 2 h before oral glucose challenge with an estimated ED_{50} of 0.8 mg/kg[1].

In the NDL2 Ptpn1 transgenic mice, PTP1B-IN-3 (compounds 3g; orally; 30 mg/kg for 21 days) shows a significant delay in the onset of tumor development in NDL2 Ptpn1$^{+/+}$ mice, extending the median tumor free days (T50) from 28 days to 75 days[1]. In diet-induced obese (DIO) mice, PTP1B-IN-3 (compounds 3g) exhibits good oral bioavailability (F of 24%), slow clearance (CL of 0.71 mL/kg/min), and good elimination half live ($t_{1/2}$ of 6 h). The oral bioavailability in higher species such as rats (F of 4%) and squirrel monkeys (F of 2%) are substantially lower but excellent exposures are achieved with oral dosing[1].

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

REFERENCES

[1]. Patel D, .Discovery of orally active, potent, and selective benzotriazole-based PTP1B inhibitors. ChemMedChem. 2011 Jun 6; 6(6):1011-6.

[2]. Yongxin Han, et al. Discovery of [(3-bromo-7-cyano-2-naphthyl)(difluoro)methyl]phosphonic acid, a potent and orally active small molecule PTP1B inhibitor. Bioorg Med Chem Lett. 2008 Jun 1;18(11):3200-5.

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