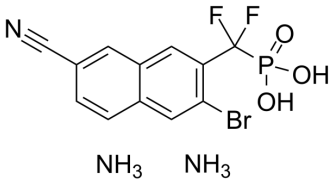
PTP1B-IN-3 diammonium

Cat. No.:	HY-15133A
CAS No.:	2702673-78-5
Molecular Formula:	$C_{12}H_{13}BrF_2N_3O_3P$
Molecular Weight:	396.12
Target:	Phosphatase
Pathway:	Metabolic Enzyme/Protease
Storage:	-20°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



BIOLOGICAL ACTIVITY

Description	PTP1B-IN-3 diammonium is a potent and orally active PTP1B inhibitor with IC_{50}s of 120 nM for both PTP1B and TCPTP. PTP1B-IN-3 diammonium 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]. Price N, et al. Safety and Efficacy of a Topical Sodium Channel Inhibitor (TV-45070) in Patients With Postherpetic Neuralgia (PHN): A Randomized, Controlled, Proof-of-Concept, Crossover Study, With a Subgroup Analysis of the Nav1.7 R1150W Genotype. Clin J Pain. 2017 Apr;33(4):310-318.

[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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