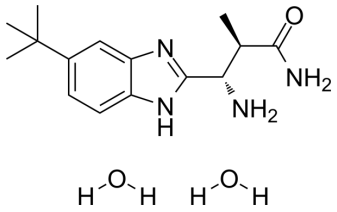
PF-06305591 dihydrate

Cat. No.:	HY-114301A
CAS No.:	2703582-76-5
Molecular Formula:	$C_{15}H_{26}N_4O_3$
Molecular Weight:	310.39
Target:	Sodium Channel
Pathway:	Membrane Transporter/Ion Channel
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (322.18 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.2218 mL	16.1088 mL	32.2175 mL
	5 mM	0.6444 mL	3.2218 mL	6.4435 mL
	10 mM	0.3222 mL	1.6109 mL	3.2218 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 (8.05 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (8.05 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (8.05 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PF-06305591 dihydrate is a potent and highly selective voltage gated sodium channel NaV1.8 blocker, with an IC_{50} of 15 nM. An excellent preclinical in vitro ADME and safety profile[1].

IC_{50} & Target

$Na_V1.8$
1.5 nM (IC_{50})

In Vitro

PF-06305591 (compound 9) has a highly attractive profile with respect to NaV selectivity, hERG activity, passive permeability and in vitro metabolic stability[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	PF-06305591 (compound 9) has good rat bioavailability. PF-06305591 offers the possibility of investigating higher IC_{50} multiples of Nav1.8 blockade in the clinic, and therefore a more thorough evaluation of the role of NaV1.8 in the treatment of pain[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Brown AD, et al. The discovery and optimization of benzimidazoles as selective NaV1.8 blockers for the treatment of pain. Bioorg Med Chem. 2019 Jan 1;27(1):230-239.

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