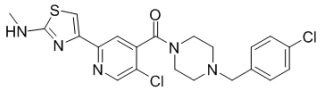
WNK-IN-11

Cat. No.:	HY-112094
CAS No.:	2123489-30-3
Molecular Formula:	$C_{21}H_{21}Cl_2N_5OS$
Molecular Weight:	462.4
Target:	Others
Pathway:	Others

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 : 150 mg/mL (**324.39 mM;** Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1626 mL	10.8131 mL	21.6263 mL
	5 mM	0.4325 mL	2.1626 mL	4.3253 mL
	10 mM	0.2163 mL	1.0813 mL	2.1626 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 (5.41 mM); Clear solution
2. Add each solvent one by one: **10% DMSO >> 90% corn oil**
   Solubility: ≥ 2.5 mg/mL (5.41 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

WNK-IN-11 is an allosteric With-No-Lysine **(WNK)** kinase inhibitor, with an **IC_{50}** of 4 nM for WNK1.

IC_{50} & Target

IC50: 4 nM (WNK1)[1].

In Vitro

WNK-IN-11 (compound 11) shows IC_{50}<2 μM in the cellular OSR1 phosphorylation assay with reasonable aqueous solubility, albeit with still rather high microsomal clearance. WNK-IN-11 shows ATP noncompetitive inhibition. When tested against a panel of 440 human kinases at 10 μM concentration, 2500-fold above enzyme IC_{50} value, WNK-IN-11 shows excellent selectivity with only a few significant off-target kinase inhibitions, most notably BTK and feline

encephalitis virus-related (FER) kinase, neither of which are implicated for blood pressure regulation. This excellent selectivity profile is consistent with the predicted allosteric binding mode outside the highly conserved ATP-pocket[1].

REFERENCES

[1]. Yamada K, et al. Optimization of Allosteric With-No-Lysine (WNK) Kinase Inhibitors and Efficacy in Rodent Hypertension Models. J Med Chem. 2017 Aug 24;60(16):7099-7107.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA