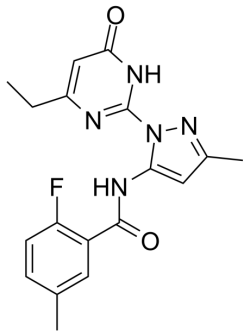
AC1-IN-1

Cat. No.:	HY-145830
CAS No.:	2762422-55-7
Molecular Formula:	$C_{18}H_{18}FN_5O_2$
Molecular Weight:	355.37
Target:	Adenylate Cyclase
Pathway:	GPCR/G Protein
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 : 25 mg/mL (70.35 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8140 mL	14.0698 mL	28.1397 mL
	5 mM	0.5628 mL	2.8140 mL	5.6279 mL
	10 mM	0.2814 mL	1.4070 mL	2.8140 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

AC1-IN-1 is a potent and selective Adenylyl cyclase type 1 (AC1) inhibitor with an IC_{50} of 0.54 μM. AC1-IN-1 displays modest antiallodynic effects in a mouse model of inflammatory pain. AC1-IN-1 has CNS activity[1].

IC_{50} & Target

IC_{50}: 0.54 μM (AC1)[1]

In Vitro

AC1-IN-1 (compound 38; HEK293 cells; 30 μM, 1 hours) shows nontoxic to this human cell line[1].

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

Cell Cytotoxicity Assay[1]

Cell Line:	HEK293 cells
Concentration:	30 μM
Incubation Time:	1 hours

Result:	Showed nontoxic to HEK293 cells.

In Vivo

AC1-IN-1 (5.6 mg/kg; i.v.) displays modest, yet statistically significant, antiallodynic effects at 1 h post-treatment compared to the 0 min (allodynic) time point[1].

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

Animal Model:	Male and female C57BL/6N mice (complete Freund's adjuvant inflammatory pain model)[1]
Dosage:	5.6 mg/kg (dissolved in 10% DMSO/10% Cremaphor/80% saline)
Administration:	Intravenous injection; 2 hours
Result:	Displayed modest, yet statistically significant, antiallodynic effects.

REFERENCES

[1]. Scott JA, et al. Optimization of a Pyrimidinone Series for Selective Inhibition of Ca2+/Calmodulin-Stimulated Adenylyl Cyclase 1 Activity for the Treatment of Chronic Pain. J Med Chem. 2022; 65(6):4667-4686.

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