SOS1-IN-15

Cat. No.: HY-151881

CAS No.: 2793404-47-2

Molecular Formula: $C_{28}H_{27}F_3N_6O_2$

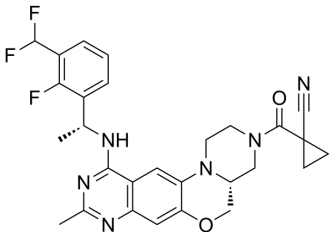
Molecular Weight: 536.55

Target: Ras

Pathway: GPCR/G Protein

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 5 mg/mL (9.32 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8638 mL	9.3188 mL	18.6376 mL
	5 mM	0.3728 mL	1.8638 mL	3.7275 mL
	10 mM	---	---	---

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

BIOLOGICAL ACTIVITY

Description

SOS1-IN-15 (Compound 37) is an orally active SOS1 inhibitor with an IC_{50} of 5 nM. SOS1-IN-15 is a promising agent candidate for the research of KRAS-driven cancer[1].

IC_{50} & Target

SOS1

5 nM (IC_{50})

In Vitro

SOS1-IN-15 (Compound 37) (0.1 nM-0.1 mM; 72 h) displays prominent inhibitory activities in Mia-paca-2 cancer cells (IC_{50} = 178 ± 42 nM)[1].

SOS1-IN-15 has a limited inhibition of CYP and hERG[1].

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

Cell Proliferation Assay[1]

Cell Line:	Mia-paca-2 pancreas cancer cells
Concentration:	0.1 nM-0.1 mM

Incubation Time:	72 h
Result:	Inhibited the proliferation with an IC_{50} of 178 ± 42 nM.

In Vivo

SOS1-IN-15 (Compound 37) (50 mg/kg; p.o.; daily for 22 days) inhibits tumor volume in mice[1].

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

Animal Model:	BALB/c nude mice bearing Mia-paca-2 pancreas tumors[1]
Dosage:	50 mg/kg
Administration:	Oral administration, daily for 22 days
Result:	Showed 49% tumor inhibition. No animal mortality and significant difference in the mice's body weight were observed during the study period.

Animal Model:	Male CD-1 Mice[1]
Dosage:	20 mg/kg
Administration:	Oral administration (Pharmacokinetic Analysis)
Result:	In Vivo Pharmacokinetic Properties of the Compounds in Male CD-1 Mice[a]

	$T_{1/2}$ (h)	T_{max} (h)	C_{max} (ng/mL)	AUC (ng⊠ h/mL)	MRT (h)	K_{el} (h^{-1})
SOS1-IN-15	11.4	3.67	1550	9900	4.19	0.25

[a]Compounds (20 mg/kg) were P.O. dosed in a mixture of 63% water + 30% PEG +5 % DMSO + 2% Tween 80 in male ICR mice (n = 3). Abbreviations: $T_{1/2}$, elimination half-life; T_{max}, plasma peak time after administration; C_{max}, maximum plasma concentration; AUC, area under concentration-time curve. MRT, mean residence time; K_{el}, elimination rate constant.

REFERENCES

[1]. Zhang S, et al. Design and Structural Optimization of Orally Bioavailable SOS1 Inhibitors for the Treatment of KRAS-Driven Carcinoma. J Med Chem. 2022 Nov 17.

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