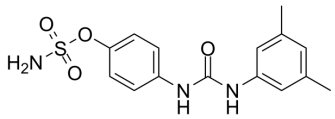
CAIX Inhibitor S4

Cat. No.:	HY-110243
CAS No.:	1330061-67-0
Molecular Formula:	$C_{15}H_{17}N_3O_4S$
Molecular Weight:	335.38
Target:	Carbonic Anhydrase
Pathway:	Metabolic Enzyme/Protease
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 : 250 mg/mL (745.42 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9817 mL	14.9085 mL	29.8169 mL
	5 mM	0.5963 mL	2.9817 mL	5.9634 mL
	10 mM	0.2982 mL	1.4908 mL	2.9817 mL

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

BIOLOGICAL ACTIVITY

Description

CAIX Inhibitor S4 is a potent and selective inhibitor of carbonic anhydrase IX/XII (CA IX/XII), with a K_i of 7 nM and 2 nM, respectively. CAIX Inhibitor S4 also inhibits CA II and CA I (K_i=546 and 5600 nM, respectively). CAIX Inhibitor S4 can inhibit the number of lung metastasis in orthotopic MDA-MB-231 mouse model without affecting primary tumor growth[1].

IC_{50} & Target

Ki: 2 nM (CA XII), 7 nM (CA IX), 546 nM (CA II), 5600 nM (CA I)[1]

In Vitro

CAIX Inhibitor S4 (1-100 μM; 24 h) inhibits the proliferation of MDA-MB-231, HCT116 and HT29 cells in a dose-dependent manner[1].

CAIX Inhibitor S4 (3.3-33 μM; 24 h) inhibits the eGFP-MDA-MB-231 cell migration in anoxia in a concentration- dependent manner[1].

CAIX Inhibitor S4 (33 μM; 15-60 min) delays the cell spreading of MDA-MB-231 cells in anoxia but essentially not in normoxia [1].

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

Cell Proliferation Assay[1]

Cell Line:	MDA-MB-231, HCT116 and HT29 cells
Concentration:	1, 10, 100 μM
Incubation Time:	24 hours
Result:	Inhibited the cell proliferation of MDA-MB-231, HCT116 and HT29 cells, with IC_{50}s of 481 μM, >1000 μM, and 20 μM, respectively.

In Vivo

CAIX Inhibitor S4 (10 mg/kg; i.p. for 14 days) inhibits metastatic tumor burden in MDA-MB-231 model while having no effect on primary tumor growth or mouse condition[1].

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

Animal Model:	Female nu/nu CBA mice (10-12 weeks) were injected with eGFP-MDA-MB-231 cells[1]
Dosage:	10 mg/kg
Administration:	I.p. daily on a “5 days on, 2 days off” dosing regimen for 14 days
Result:	Significantly reduced the metastatic tumor burden in lungs of mice bearing orthotopic eGFP-MDA-MB-231 tumors. The average body weights between vehicle and S4 treated mice were similar throughout the experiments.

REFERENCES

[1]. Gieling RG, et, al. Antimetastatic effect of sulfamate carbonic anhydrase IX inhibitors in breast carcinoma xenografts. J Med Chem. 2012 Jun 14;55(11):5591-600.

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