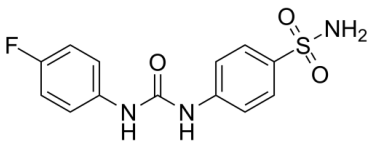
Data Sheet

Product Name:	U-104
Cat. No.:	CS-4495
CAS No.:	178606-66-1
Molecular Formula:	$C_{13}H_{12}FN_3O_3S$
Molecular Weight:	309.32
Target:	Carbonic Anhydrase
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 100 mg/mL (323.29 mM)



BIOLOGICAL ACTIVITY:

U-104 (SLC-0111) is a potent **carbonic anhydrase (CA)** inhibitor for CA IX and CA XII with **K_i** values of 45.1 nM and 4.5 nM, respectively. U-104 shows a significant delay in tumor growth in mice model[1][2]. IC50 & Target: Ki: 45.1 nM (CA IX) and 4.5 nM (CA XII)[1]

EC50: 0.2 μM (exosome)[3] **In Vitro:** U-104 (SLC-0111) is a potent exosome inhibitor[3].

U-104 has low inhibition for CA I (K_i=5080 nM) and CA II (K_i=9640 nM)[1].

U-104 (50 μM; for 72 hours) blocks the mesenchymal phenotype in the cancer stem cells population in hypoxia condition of 4T1 cells.

U-104 (<50 μM) significantly reduces migration in a dose-dependent manner in metastatic MDA-MB-231 LM2-4^{Luc+} cells , with cells growing as compact colonies similar to parental MDA-MB-231 cells[2]. **In Vivo:** U-104 (19, 38 mg/kg; daily; for 27 days) inhibits primary tumor growth in the mice implanted orthotopically with MDA-MB-231 LM2-4Luc+ cells. U-104 (19 mg/kg; daily; for 5 days) inhibits metastases formation in the 4T1 experimental metastasis mice model[1].

U-104 (38 mg/kg; i.p.; from 11 to 27 days) significantly delays primary tumor growth and reduces cancer stem cell population in NOD/SCID mice orthotopically implanted with MDA-MB-231 LM2-4^{Luc+} cells[2].

U-104 (50 mg/kg; oral gavage; continuously for 4 days and suspended for 1 day; from 10 to 30 days) shows a significant delay in tumor growth in Balb/c mice orthotopically implanted with 4T1 cells[2].

PROTOCOL (Extracted from published papers and Only for reference)

in vivo study [1] For in vivo studies, CAI17, ureido-sulfonamide U-104, and glycosyl coumarins GC-204 and GC-205 were solubilized in 37.5% PEG400/12.5% ethanol/50% saline prior to injection. Drug aliquots were made fresh daily or were prepared, frozen at 80°C in single-use aliquots, and thawed prior to administration. Drugs were administered by i.p. injection, except for CAI17, in which the first 2 doses were administered by i.v. injection, followed by i.p. injection of the remaining doses. Specific dosing schedules are described in the appropriate figures.

References:

[1]. Lou Y, et al. Targeting tumor hypoxia: suppression of breast tumor growth and metastasis by novel carbonic anhydrase IX inhibitors. Cancer Res. 2011 May 1;71(9):3364-76.

[2]. Lock FE, et al. Targeting carbonic anhydrase IX depletes breast cancer stem cells within the hypoxic niche. Oncogene. 2013 Oct 31;32(44):5210-9.

[3]. Huarui Zhang, et al. Advances in the discovery of exosome inhibitors in cancer. J Enzyme Inhib Med Chem. 2020 Dec;35(1):1322-1330.

CAIndexNames:

Benzenesulfonamide, 4-[[[(4-fluorophenyl)amino]carbonyl]amino]-

SMILES:

O=S(C1=CC=C(NC(NC2=CC=C(F)C=C2)=O)C=C1)(N)=O

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