U-104

Cat. No.: HY-13513

CAS No.: 178606-66-1

Molecular Formula: $C_{13}H_{12}FN_3O_3S$

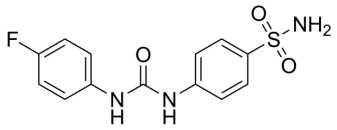
Molecular Weight: 309.32

Target: Carbonic Anhydrase

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	1 year
	-20°C	6 months



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (323.29 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.2329 mL	16.1645 mL	32.3290 mL
5 mM	0.6466 mL	3.2329 mL	6.4658 mL
10 mM	0.3233 mL	1.6164 mL	3.2329 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: ≥ 2.08 mg/mL (6.72 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (6.72 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (6.72 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

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].

IC_{50} & Target		
	CA XII	CA ⊠

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

CUSTOMER VALIDATION

- Anal Chem. 2023 Feb 1.
- bioRxiv. 2023 Sep 8.
- Oxid Med Cell Longev. 2023 Jan 31.

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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.

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