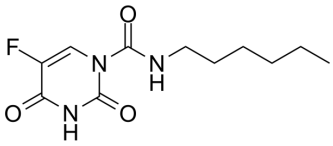
Carmofur

Cat. No.: HY-B0182

CAS No.: 61422-45-5

Molecular Formula: $C_{11}H_{16}FN_3O_3$

Molecular Weight: 257.26



Target: Nucleoside Antimetabolite/Analog; SARS-CoV; Virus Protease; FAAH; Ceramidase; Glutathione Peroxidase

Pathway: Cell Cycle/DNA Damage; Anti-infection; Metabolic Enzyme/Protease; Neuronal Signaling; Apoptosis

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 : 83.33 mg/mL (323.91 mM; Need ultrasonic)

H_2O : 0.67 mg/mL (2.60 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.8871 mL	19.4356 mL	38.8712 mL
	5 mM	0.7774 mL	3.8871 mL	7.7742 mL
	10 mM	0.3887 mL	1.9436 mL	3.8871 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 (8.09 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (8.09 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (8.09 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Carmofur (HCFU) is a rat recombinant acid ceramidase inhibitor with an IC_{50} of 29 nM. Carmofur is also a protease inhibitor of SARS-CoV-2 main protease (Mpro), fatty acid amide hydrolase (FAAH) and N-acylethanolamine acid amidase (NAAA). Carmofur has anti-cancer, anti-inflammatory and anti-virus activities, and can be used for the study of COVID-19 and acute lung injury (ALI)[1][2][3].

IC_{50} & Target	IC50: 29 nM (acid ceramidase)[1]. N-Acylethanolamine Acidase (NAAA)[3].

In Vitro

Carmofur (0.3-10 μM; 20 min-1 h) inhibits acid ceramidase (AC) activity in a concentration- and time-dependent manner in human colon cancer SW403 cells[1].
Carmofur (1-100 μM) inhibits he activity of SARS-CoV-2 with an EC_{50} of 24.3 μM in Vero E6 cells[2].
Carmofur (5 μM; 6 h) inhibits the activities of FAAH and NAAH with IC_{50} values of 0.11 μM and 0.71 μM, respectively, in HEK293 cells[3].
Carmofur (10 μM; 30 min) has anti-inflammatory activity in Raw264.7 cells[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Real Time qPCR[3]

Cell Line:	Raw264.7
Concentration:	10 μM. After LPS treatment (500 ng/mL; 72 h)
Incubation Time:	30 min
Result:	Effectively reduced the mRNA expression of pro-inflammatory cytokines such as IL-1β, IL-6, iNOS, TNF-α.

Western Blot Analysis[3]

Cell Line:	Raw264.7
Concentration:	1 μM, 3 μM, 10 μM. After LPS treatment (500 ng/mL; 72 h)
Incubation Time:	30 min
Result:	Down-regulated the expression levels of p-p65 and p-κbα proteins in a dose-dependent manner, blocking the nuclear translocation of p65.

In Vivo

Carmofur (10-30 mg/kg; Intraperitoneal injection (I.P.), single dose) inhibits acid ceramidase (AC) activity in various tissues, including lung and cerebral cortex, in male Swiss Webster mice[1].
Carmofur (10 mg/kg; P.O. , single dose) significantly improves the LPS- (5 mg/kg; tracheal perfusion, single dose) (HY-D1056) induced inflammatory response by inhibiting the activities of FAAH and NAAA in in acute lung injury (ALI) mice, promoting the resolution of lung injury[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male C57BL/6J mice model of LPS-induced ALI[3]
Dosage:	3 mg/kg, 10 mg/kg
Administration:	Oral gavage (p.o.), single dose. After LPS treatment (5 mg/kg; Tracheal perfusion, single dose)
Result:	Significantly inhibited MPO activity, which is a marker of neutrophil abundance. Alleviated alveolar edema and inhibited neutrophil accumulation.

CUSTOMER VALIDATION

- ACS Cent Sci. February 2, 2022.
- Nucleic Acids Res. 2021 Jan 8;49(D1):D1113-D1121.

- J Mol Med (Berl). 2019 Aug;97(8):1183-1193.

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REFERENCES

[1]. Jin Z, et al. Structural basis for the inhibition of SARS-CoV-2 main protease by antineoplastic drug carmofur. Nat Struct Mol Biol. 2020 Jun;27(6):529-532.

[2]. Realini N, Solorzano C, Pagliuca C, et al. Discovery of highly potent acid ceramidase inhibitors with in vitro tumor chemosensitizing activity[J]. Scientific reports, 2013, 3(1): 1035.

[3]. Wu K, et al. A new use for an old drug: carmofur attenuates lipopolysaccharide (LPS)-induced acute lung injury via inhibition of FAAH and NAAA activities[J]. Frontiers in pharmacology, 2019, 10: 818.

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