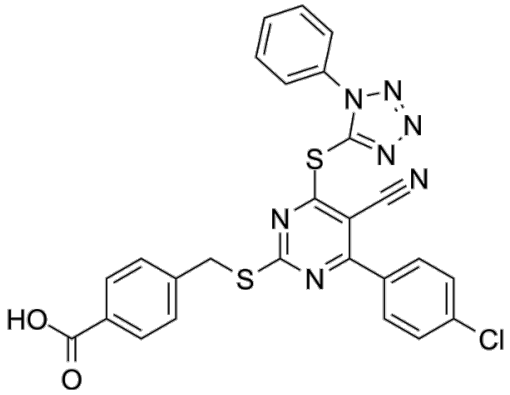
Product Data Sheet

Product Name: SHMT2-IN-1
Cat. No.: GC81596

Chemical Properties

Cas. No.			
Formula	$C_{26}H_{16}ClN_7O_2S_2$	M.Wt	558.03
Solubility	DMSO: 100 mg/mL (179.20 mM; ultrasonic and warming and heat to 60°C)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		

Structure



Background

SHMT2-IN-1 is a potent serine hydroxymethyltransferase 2 (SHMT2) inhibitor with an IC_{50} of 1.21 μM and a K D of 10.6 μM. SHMT2-IN-1 binds to the folate binding site of SHMT2. SHMT2-IN-1 also inhibits SHMT1 with an IC_{50} of 1.83 μM. SHMT2-IN-1 can inhibit cancer cells proliferation, migration and invasion. SHMT2-IN-1 can induce cells apoptosis and ROS production and cause G2/M phase arrest. SHMT2-IN-1 can be used for the research of cancer, such as esophageal cancer [1].

Caution: Product has not been fully validated for medical applications. For research use only.
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In Vitro, SHMT2-IN-1 (0.1-10 μM, 24 h) exhibits potent antiproliferative activity against esophageal cancer cells KYSE-450 and KYSE-70 with IC_{50} values of 1.62 μM and 1.18 μM respectively [1]. SHMT2-IN-1 (2.5-10 μM, 24 h) dose-dependently inhibits the migration and invasion of KYSE-450 and KYSE-70 cells[1]. SHMT2-IN-1 (2.5-7.5 μM, 24-72 h) induces apoptosis, ROS production and cause G2/M phase arrest in KYSE-450 and KYSE-70 cells[1].

References:

[1]. Akram HMB, et al. Discovery of W478, a novel SHMT2 inhibitor for the treatment of esophageal carcinoma. Bioorg Chem. 2025 Oct;165:109028.

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