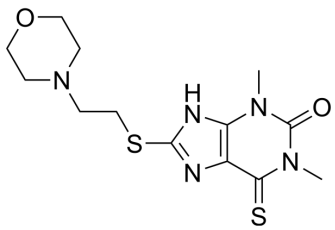
JA2131

Cat. No.:	HY-137924
CAS No.:	6505-99-3
Molecular Formula:	$C_{13}H_{19}N_5O_2S_2$
Molecular Weight:	341.45
Target:	Poly(ADP-ribose) Glycohydrolase (PARG)
Pathway:	Cell Cycle/DNA Damage
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 : 12.5 mg/mL (36.61 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9287 mL	14.6434 mL	29.2869 mL
	5 mM	0.5857 mL	2.9287 mL	5.8574 mL
	10 mM	0.2929 mL	1.4643 mL	2.9287 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (3.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

JA2131 is a small molecular inhibitor of Poly(ADP-ribose) Glycohydrolase (PARG) (IC_{50}=0.4 μM). JA2131 regulate DNA damage responses, causes replication fork stalling and cancer cell death[1][2].

In Vitro

JA2131 (10 mM; 1-2 h) induces hyperPARylation of PARP1 in PC3 cells[1].
JA2131 (10 μM; 2 wk) inhibits colony formation of MCF-7, PC3, and MDA-MB-231 cells, and (0.1 μM-1 mM; 72 h) shows cytotoxicity to inhibit MRC-50 cells with an IC_{50} value of 132 μM[1].
JA2131 (5 μM; 72 h) inhibits PC3, and A172 glioblastoma cells viability[1].
JA2131 (10 μM; 2 h) could be acting at the replication fork in HeLa cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	PC3, and A172 glioblastoma cells
Concentration:	0.1 μM-10 mM
Incubation Time:	72 hours
Result:	Inhibited cell viability with IC50s of 33.05 μM (PC3 cells) and 55.34 μM (A172 cells), respectively.

REFERENCES

[1]. Houl JH, et al. Selective small molecule PARG inhibitor causes replication fork stalling and cancer cell death. Nat Commun. 2019 Dec 11;10(1):5654.

[2]. Brosey CA, et al. Targeting SARS-CoV-2 Nsp3 macrodomain structure with insights from human poly(ADP-ribose) glycohydrolase (PARG) structures with inhibitors. Prog Biophys Mol Biol. 2021 Aug;163:171-186.

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