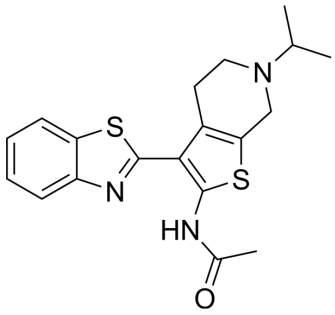
APE1-IN-1

Cat. No.:	HY-136731
CAS No.:	524708-03-0
Molecular Formula:	$C_{19}H_{21}N_3OS_2$
Molecular Weight:	371.52
Target:	DNA/RNA Synthesis
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 : 22 mg/mL (59.22 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6916 mL	13.4582 mL	26.9165 mL
	5 mM	0.5383 mL	2.6916 mL	5.3833 mL
	10 mM	0.2692 mL	1.3458 mL	2.6916 mL

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

BIOLOGICAL ACTIVITY

Description

APE1-IN-1 is a potent and blood-brain barrier (BBB) penetrant apurinic/apyrimidinic (AP) endonuclease 1 (APE1) inhibitor with an IC_{50} value of 2 μM. APE1-IN-1 can potentiate the cytotoxicity of the alkylating agents Methylmethane sulfonate and Temozolomide (HY-17364) to cancer cells[1].

IC_{50} & Target

IC_{50}: 2 μM (APE1)[1]

In Vitro

APE1-IN-1 (compound 3) exhibits an IC_{50} of 2 μM in the qHTS assay and an IC_{50} of 12 μM in a radiotracer incision assay (RIA)[1].

APE1-IN-1 (0, 1, 3, 10, 30, or 100 μM; 15 min) inhibits HeLa whole cell extract AP site incision in a dose-dependent manner[1].

APE1-IN-1 (5-30 μM; 24 h) exhibits cytotoxic activity against HeLa cells, and potentiates the activity of methyl methansulfonate and Temozolomide (HY-17364)[1].

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

Cell Cytotoxicity Assay[1]

Cell Line:	HeLa cells
Concentration:	5-30 μM
Incubation Time:	24 h
Result:	Exhibited cytotoxic activity against HeLa cells with a 50% reduction in cell viability occurring at ~15 μM. Greatly potentiated the activity of methyl methansulfonate (0.4 mM) and Temozolomide (HY-17364) (1 mM) with optimal synergy occurring at ~5 μM and ~10 μM, respectively.

In Vivo

APE1-IN-1 (30 mpk; IP; single dosage) exhibits favorable pharmacokinetic property[1].

Pharmacokinetic Parameters of APE1-IN-1 (compound 3) (IP; 30 mpk) in CD1 mice[1].

	Plasma	Brain
$t_{1/2}$ (h)	2.1	1
brain/plasma	21	
C_{max} (μM)	16	217
t_{max} (h)	0.25	0.25
CLogP	2.83	

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

Animal Model:	CD1 male mice (n = 3)[1]
Dosage:	30 mpk
Administration:	IP; single dosage
Result:	Showed lipophilic (CLogP = 2.8), crossed the BBB quite readily, giving rise to a B/P ratio of 21.

REFERENCES

[1]. Rai G, et al. Synthesis, biological evaluation, and structure-activity relationships of a novel class of apurinic/apyrimidinic endonuclease 1 inhibitors. J Med Chem. 2012 Apr 12;55(7):3101-12.

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