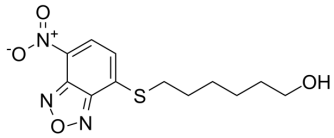
NBDHEX

Cat. No.:	HY-135318
CAS No.:	787634-60-0
Molecular Formula:	$C_{12}H_{15}N_3O_4S$
Molecular Weight:	297.33
Target:	Glutathione Peroxidase; Apoptosis; Autophagy
Pathway:	Metabolic Enzyme/Protease; Apoptosis; Autophagy
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (420.41 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.3633 mL	16.8163 mL	33.6327 mL
	5 mM	0.6727 mL	3.3633 mL	6.7265 mL
	10 mM	0.3363 mL	1.6816 mL	3.3633 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 (7.00 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (7.00 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NBDHEX is a potent glutathione S-transferase P1-1 (GSTP1-1) inhibitor. NBDHEX induces apoptosis of tumor cells. NBDHEX acts as an anticancer agent by inhibiting GSTs catalytic activity, avoiding inconvenience of the inhibitor extrusion from the cell by specific pumps and disrupting the interaction between the GSTP1-1 and key signaling effectors. NBDHEX can also act as late-phase autophagy inhibitor[1][2].

IC_{50} & Target

Glutathione S-transferase P1-1 (GSTP1-1)[1];
Apoptosis[1];
Autophagy[1]

In Vitro

NBDHEX (0.05-20 μM; 48 hours; H69 and H69AR cells) is cytotoxic toward cell lung cancer H69 and H69AR cells[2].

NBDHEX (0-5 μM; 24 hours; H69AR cells) treatment results in a dose-dependent apoptosis in the H69AR cell line[2].
NBDHEX (3 μM; 1-12 hours; H69AR cells) treatment increases the phosphorylation of JNK/c-Jun in H69AR cells in a time-dependent fashion[2].
NBDHEX treatment shows a marked increase in phosphorylation of $p38^{MAPK}$, and also increases GSSG content in a time-dependent manner in H69 cells[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[2]

Cell Line:	H69 and H69AR cells
Concentration:	0.05-20 μM
Incubation Time:	48 hours
Result:	The dose-response profiles revealed a good cytotoxic activity both in sensitive H69 cell line (LC_{50} of 2.3 μM) and in its Adriamycin-resistant counterpart H69AR (LC_{50} of 4.5 μM).

Apoptosis Analysis[2]

Cell Line:	H69AR cells
Concentration:	0 μM, 0.5 μM, 1 μM, 2 μM, 3 μM, 4 μM, 5 μM
Incubation Time:	24 hours
Result:	Resulted in a dose-dependent apoptosis in the H69AR cell line.

Western Blot Analysis[2]

Cell Line:	H69AR cells
Concentration:	3 μM
Incubation Time:	1 hour,3 hours, 6 hours, 12 hours
Result:	Increased the phosphorylation of JNK/c-Jun in H69AR cells in a time-dependent fashion.

In Vivo

NBDHEX (0.8-80 mg/kg/day; oral administration; daily; for 15 days; SCID female mice) treatment results a statistically significant tumour inhibition (approximately 70%)[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	SCID female mice (4-5 weeks) injected with Me501cells[3]
Dosage:	0.8 mg/kg/day, 8.0 mg/kg/day or 80 mg/kg/day
Administration:	Oral administration; daily; for 15 days
Result:	A statistically significant tumour inhibition (approximately 70%) was observed.

CUSTOMER VALIDATION

- Reprod Sci. 2023 Mar 16.

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REFERENCES

[1]. Sha HH, et al. 6-(7-nitro-2,1,3-benzoxadiazol-4-ylthio) hexanol: a promising new anticancer compound. Biosci Rep. 2018 Feb 13;38(1). pii: BSR20171440.

[2]. Filomeni G, et al. 6-(7-Nitro-2,1,3-benzoxadiazol-4-ylthio)hexanol, a specific glutathione S-transferase inhibitor, overcomes the multidrug resistance (MDR)-associated protein 1-mediated MDR in small cell lung cancer. Mol Cancer Ther. 2008 Feb;7(2):371-9

[3]. Pellizzari Tregno F, et al. In vitro and in vivo efficacy of 6-(7-nitro-2,1,3-benzoxadiazol-4-ylthio)hexanol (NBDHEX) on human melanoma. Eur J Cancer. 2009 Sep;45(14):2606-17.

Caution: Product has not been fully validated for medical applications. For research use only.

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