

Product data sheet



MedKoo Cat#: 462531 Name: NBDHEX CAS: 787634-60-0 Chemical Formula: C ₁₂ H ₁₅ N ₃ O ₄ S Exact Mass: 297.0783 Molecular Weight: 297.329	
Product supplied as: Powder	
Purity (by HPLC): ≥ 98%	
Shipping conditions: Ambient temperature	
Storage conditions: Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

1. Product description:

NBDHEX is a potent glutathione S-transferase P1-1 (GSTP1-1) inhibitor. It 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.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	125.0	420.41

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.63 mL	16.82 mL	33.63 mL
5 mM	0.67 mL	3.63 mL	6.73 mL
10 mM	0.34 mL	1.68 mL	3.36 mL
50 mM	0.07 mL	0.34 mL	0.67 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

- Liu W, Cheng L, Du Y, Liu X, Ma J, Yan L. 6-(7-Nitro-2,1,3-benzoxadiazol-4-ylthio) Hexanol Inhibits Proliferation and Induces Apoptosis of Endometriosis by Regulating Glutathione S-Transferase Mu Class 4. *Reprod Sci.* 2023 Mar 16. doi: 10.1007/s43032-023-01207-x. Epub ahead of print. PMID: 36928896.
- Filomeni G, Turella P, Dupuis ML, Forini O, Ciriolo MR, Cianfriglia M, Pezzola S, Federici G, Caccuri AM. 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. doi: 10.1158/1535-7163.MCT-07-0487. PMID: 18281520.

In vivo study

- Sha H, Dong S, Yu C, Zou R, Zhu Y, Lu Y, Zhang J, Cao H, Chen D, Wu J, Feng J. In Vitro and in Vivo Efficacy of NBDHEX on Gefitinib-resistant Human Non-small Cell Lung Cancer. *J Cancer.* 2020 Oct 18;11(24):7216-7223. doi: 10.7150/jca.46461. PMID: 33193885; PMCID: PMC7646187.
- Pellizzari Tregno F, Sau A, Pezzola S, Geroni C, Lapenta C, Spada M, Filomeni G, Bonanno E, Federici G, Caccuri AM. 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. doi: 10.1016/j.ejca.2009.06.033. Epub 2009 Aug 6. PMID: 19665369.

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7. Bioactivity

Biological target:

NBDHEX is a potent glutathione S-transferase P1-1 (GSTP1-1) inhibitor.

In vitro activity

Interestingly, NBDHEX triggers two different types of cell death: a caspase-dependent apoptosis in the H69AR cells and a necrotic phenotype in the parental H69 cells. The apoptotic pathway triggered by NBDHEX in H69AR cells is associated with c-Jun NH(2)-terminal kinase and c-Jun activation, whereas glutathione oxidation and activation of p38(MAPK) is observed in the NBDHEX-treated H69 cells.

Reference: Mol Cancer Ther. 2008 Feb;7(2):371-9. <https://pubmed.ncbi.nlm.nih.gov/18281520/>

In vivo activity

The in vivo antitumour efficacy of NBDHEX was evaluated on human melanoma (Me501 and A375) mouse models. After 15 d of daily treatment, a statistically significant tumour inhibition (approximately 70%) was observed (Fig. 7, panel A). Tumours treated with NBDHEX showed a more than 50% decrease in the mitotic index (Fig. 7, panel C).

Reference: Eur J Cancer. 2009 Sep;45(14):2606-17. <https://pubmed.ncbi.nlm.nih.gov/19665369/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.