

Product Data Sheet

Product Name: Benitrobenrazide (Hexokinase 2 inhibitor 1)

Cat. No.: GC70717

Chemical Properties

Cas. No. 2454676-05-0

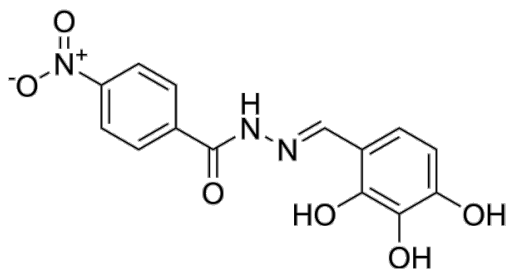
Formula $C_{14}H_{11}N_3O_6$ M.Wt 317.25

Solubility DMSO : 125 mg/mL (394.01 mM); Storage -20°C
Need ultrasonic; Hygroscopic DMSO has a significant impact on the solubility of product, please use newly opened DMSO)

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



Protocol

Cell experiment [1]:

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

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Cell lines	Hu1545 human hepatocyte cell line (derived from human Telomerase Reverse Transcriptase (hTERT)-mediated immortalization)
Preparation Method	Hu1545 cells were treated with palmitate (PA) at 400μM with or without the selective Benitrobenrazide (10μM or 30μM).
Reaction Conditions	10μM or 30μM; 8h.
Applications	Benitrobenrazide significantly attenuated palmitate-induced lipid droplet accumulation (steatosis).

Animal experiment [2]:

Animal models	BALB/c nude mice bearing MDA-MB-231 tumor xenografts
Preparation Method	Benitrobenrazide was administered orally to tumor-bearing mice.
Dosage form	200mg/kg; p.o.; once daily for 21 days.
Applications	Benitrobenrazide significantly inhibited tumor growth and did not cause obvious toxicity.

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References:

- [1] Daniel PV, Puri G, Luo Y, et al. Silencing of S100A11 attenuates murine metabolic dysfunction-associated steatohepatitis. NPJ Gut Liver. 2025;2(1):32.
- [2] Zheng M, Wu C, Yang K, et al. Novel selective hexokinase 2 inhibitor Benitrobenrazide blocks cancer cells growth by targeting glycolysis. Pharmacol Res. 2021 Feb;164:105367.

Background

Benitrobenrazide (Hexokinase 2 inhibitor 1) inhibits glycolysis by directly targeting HK2. Benitrobenrazide can induce apoptosis and promote the production of reactive oxygen species to inhibit cancer cell proliferation. Benitrobenrazide can be used in research related to pancreatic cancer and colorectal cancer^[1-4].

In vitro, HepG2 and HUH7 human liver cancer cells were treated with Benitrobenrazide (15 μ M or 57.1 μ M) for 72 hours. Benitrobenrazide caused DNA damage, increased reactive oxygen species (ROS) production, and disrupted cell cycle progression. Its inhibitory effect may be related to HK2 inhibition and compound aggregation effects^[1]. The Hu1545 human hepatocyte cell line was co-treated with Benitrobenrazide (10 μ M or 30 μ M) and 400 μ M palmitate for 8 hours. Benitrobenrazide significantly attenuated palmitate-induced lipid droplet accumulation (steatosis)^[2].

In vivo, Benitrobenrazide (200mg/kg) was administered orally once daily for 21 days to BALB/c nude mice bearing MDA-MB-231 tumor xenografts. Benitrobenrazide significantly inhibited tumor growth and did not cause obvious toxic reactions^[3].

References:

- [1] Juszczak K, Kubicka A, Kitel R, et al. Hexokinase 2 Inhibition and Biological Effects of BNBZ and Its Derivatives: The Influence of the Number and Arrangement of Hydroxyl Groups. Int J Mol Sci. 2022 Feb 27;23(5):2616.
- [2] Daniel PV, Puri G, Luo Y, et al. Silencing of S100A11 attenuates murine metabolic dysfunction-associated steatohepatitis. NPJ Gut Liver. 2025;2(1):32.
- [3] Zheng M, Wu C, Yang K, et al. Novel selective hexokinase 2 inhibitor Benitrobenrazide blocks cancer cells growth by targeting glycolysis. Pharmacol Res. 2021 Feb;164:105367.
- [4] Al-Jabiri MH, Anshasi MA, Ma J, et al. Shapes of Benzyl Benzoate: A Rotational Spectroscopic

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and Computational Study. J Phys Chem A. 2026 Mar 19;130(11):2443-2450.

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