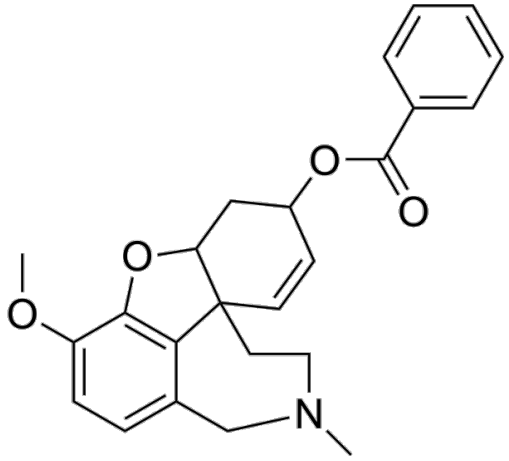
Product Data Sheet

Product Name: HK2-IN-4
Cat. No.: GC79709

Chemical Properties

Cas. No.	2748366-80-3		
Formula	$C_{24}H_{25}NO_4$	M.Wt	391.46
Solubility	DMSO: 100 mg/mL (255.45 mM; Need ultrasonic)	Storage	Store at 4°C, protect from light
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



Background

Product Data Sheet

HK2-IN-4 is a selective hexokinase 2 (HK2) inhibitor with an IC_{50} value of 0.79 μM and a K d value of 0.41 μM. HK2-IN-4 blocks the interaction between HK2 and voltage-dependent anion channel 1 (VDAC1). HK2-IN-4 reduces lactate and ATP levels in cancer cells. HK2-IN-4 induces the production of apoptosis (apoptosis) markers in cancer cells, including increased p-AMPK/AMPK ratio and Bax levels, as well as decreased Bcl2 levels. HK2-IN-4 inhibits the proliferation of cancer cells with high HK2 expression. HK2-IN-4 can be used in research related to colorectal cancer and non-small cell lung cancer [1].

In Vitro, HK2-IN-4 (Compound 106) (5 μM; 30 min) potently and selectively inhibits the activity of recombinant HK2 enzyme, with an IC_{50} of 0.79 μM, while its IC_{50} values against HK1, HK3 and HK4 are 78.47 μM, 60.86 μM and 46.14 μM, respectively[1]. HK2-IN-4 (10-100 μM; 24-72 h) selectively inhibits the viability of colorectal cancer cells with high HK2 expression (SW480, LOVO, HCT116), with an IC_{50} value as low as 5.00 μM after 72 h under hypoxic conditions; compared with normoxic conditions, its efficacy is enhanced under hypoxic conditions, and its cytotoxicity depends on HK2 expression[1]. HK2-IN-4 (0-40 μM; 6 h) reduces mitochondrial HK2 levels in HCT116 and SW480 cells in a dose-dependent manner under hypoxic conditions[1]. Treatment with HK2-IN-4 (50 μM; 7 h) significantly reduces the colocalization level of HK2 and VDAC1 in SW480 cells and disrupts the HK2-VDAC1 interaction[1]. HK2-IN-4 (50-100 μM; 2 h) inhibits glycolysis in SW480 and HCT116 WT cells under hypoxic conditions, but exerts no such effect on HK2 KO cells, indicating that its glycolysis-inhibiting effect is HK2-dependent[1]. HK2-IN-4 (2.5-20 μM; 12-24 h) reduces lactate and ATP levels in hypoxic SW480 colorectal cancer cells in a dose-dependent manner, increases the p-AMPK/AMPK ratio, regulates the expression levels of Bax/Bcl2, and induces bioenergetic stress and apoptosis[1].

References:
[1]. Shan W, et al. AI-driven identification of a selective dual function inhibitor blocking HK2 activity and HK2-VDAC1 interaction displaying enhanced anticancer efficacy under hypoxia. Eur J Med Chem. 2026;309:118752.

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