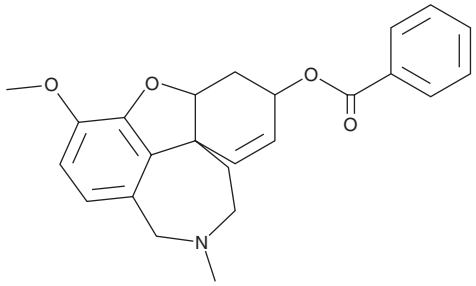
PRODUCT INFORMATION

HK2-IN-4

Item No. 46754

CAS Registry No.:	2748366-80-3
Formal Name:	4a,5,9,10,11,12 hexahydro-3-methoxy-11-methyl-6H-benzofuro[3a,3,2-ef][2] benzazepin-6-ol, 6-benzoate
Synonyms:	HK2 Inhibitor 4, Hexokinase-2-IN-4, Hexokinase-2 Inhibitor 4
MF:	$C_{24}H_{25}NO_4$
FW:	391.5
Purity:	≥95%
Supplied as:	A solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

HK2-IN-4 is supplied as a solid. A stock solution may be made by dissolving the HK2-IN-4 in the solvent of choice, which should be purged with an inert gas. HK2-IN-4 is soluble (≥10 mg/ml) in ethanol and DMSO.

Description

HK2-IN-4 is an inhibitor of hexokinase-2 (HK2; IC_{50} = 0.79 µM).[1] It is selective for HK2 over HK1, HK3, and HK4 (IC_{50}s = 78.5, 60.9, and 46.1 µM, respectively). HK2-IN-4 is selectively cytotoxic to SW480, LoVo, and HCT116 colorectal cancer cells grown under hypoxic conditions (IC_{50}s = 5, 11.1, and 16.2 µM, respectively) over the same cells grown under normoxic conditions (IC_{50}s = 14.3, 27.1, and 43.3 µM, respectively). It reduces lactate and ATP levels and induces apoptosis in SW480 cells.

Reference

1. Shan, W., Zhang, S.L., Assaraf, Y.G., *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.* **309**, 118752 (2026).

WARNING
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA
This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent *via* email to your institution.

WARRANTY AND LIMITATION OF REMEDY
Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 11/12/2026

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM