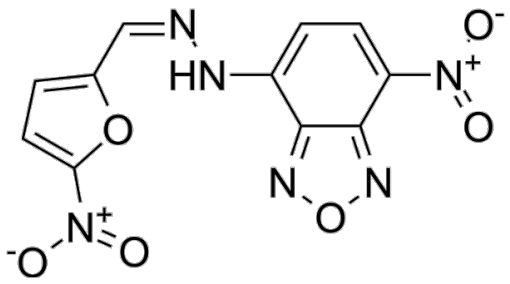
Product Data Sheet

Product Name: PFKFB4-IN-1
Cat. No.: GC79577

Chemical Properties

Cas. No.	2664831-55-2		
Formula	$C_{11}H_6N_6O_6$	M.Wt	318.2
Solubility	DMSO: 20 mg/mL (62.85 mM; Need ultrasonic and warming)	Storage	Store at 4°C, away from moisture
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

PFKFB4-IN-1 is a potent and selective ATP-competitive PFKFB4 inhibitor (IC_{50} = 4.50 μM) that reduces intracellular PFKFB4 protein levels. PFKFB4-IN-1 exhibits >12-fold selectivity over PFKFB1/4 and PFKFB3/4. PFKFB4-IN-1 inhibits cancer cell proliferation, induces apoptosis, and inhibits cell migration. PFKFB4-IN-1 inhibits tumor growth in the MDA-MB-231 xenograft mouse model. PFKFB4-IN-1 can be used for breast, lung and liver cancer research [1].

In Vivo, PFKFB4-IN-1 (30 mg/kg, i.p., q.d. for 14 days) inhibits tumor growth in MDA-MB-231

xenograft mouse model[1]. PFKFB4-IN-1 (5 μM, a single dose at 24 h post-fertilization for 72 h) shows a favorable acute safety profile in the zebrafish developmental toxicity model[1].

In Vitro, PFKFB4-IN-1 (compound 2v) (2-100 μM, 72 h) demonstrates broad-spectrum anticancer activity, with IC_{50} values of 4.02 μM (MCF-7), 11.07 μM (HepG2), and 11.2 μM (A549), while showing significantly lower cytotoxicity toward normal human liver cells (HL7702, IC_{50} > 50 μM)[1]. PFKFB4-IN-1 (0-48 h) inhibits proliferation of MCF-7 breast cancer cells in both time- and concentration-dependent manner[1]. PFKFB4-IN-1 (6-18 μM, 24 h) inhibits both migration and colony formation, and induces apoptosis in MCF-7 breast cancer cells through the canonical caspase-3 activation and PARP cleavage pathway[1]. PFKFB4-IN-1 (0-25 μM, 24 h) suppresses PFKFB4 protein levels and suppresses glycolytic metabolism in MCF-7 cells, with markedly reduced intracellular ATP and NADP+/NADPH levels[1]. PFKFB4-IN-1 stably binds within the ATP-binding pocket of PFKFB4, forming key hydrogen bonds with residues Asn168, Gly51, and Tyr428. PFKFB4-IN-1 shows no significant increase in ROS levels and DNA damage in MCF-7 cells[1].

References:
[1]. Chen Y, et al. Structure-guided discovery of nitrobenzo-2-oxa-1,3-diazole (NBD) scaffold-based PFKFB4 inhibitors for cancer therapy. Eur J Med Chem. 2025 Dec 15;300:118109.