

## Product Data Sheet

Product Name: PFKFB4-IN-1

Cat. No.: GC79577

### Chemical Properties

Cas. No. 2664831-55-2

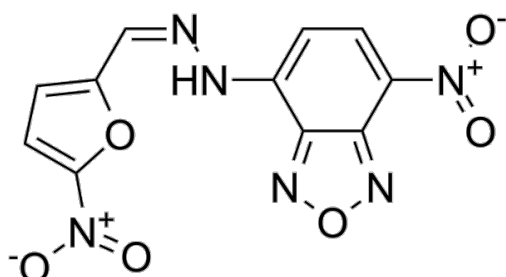
Formula  $C_{11}H_6N_6O_6$  M.Wt 318.2

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 ( $IC_{50} = 4.50 \mu M$ ) 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

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

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xenograft mouse model<sup>[1]</sup>. PFKFB4-IN-1 (5  $\mu$ M, a single dose at 24 h post-fertilization for 72 h) shows a favorable acute safety profile in the zebrafish developmental toxicity model<sup>[1]</sup>.

In Vitro, PFKFB4-IN-1 (compound 2v) (2-100  $\mu$ M, 72 h) demonstrates broad-spectrum anticancer activity, with IC<sub>50</sub> values of 4.02  $\mu$ M (MCF-7), 11.07  $\mu$ M (HepG2), and 11.2  $\mu$ M (A549), while showing significantly lower cytotoxicity toward normal human liver cells (HL7702, IC<sub>50</sub> > 50  $\mu$ M)<sup>[1]</sup>. PFKFB4-IN-1 (0-48 h) inhibits proliferation of MCF-7 breast cancer cells in both time- and concentration-dependent manner<sup>[1]</sup>. PFKFB4-IN-1 (6-18  $\mu$ M, 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<sup>[1]</sup>. PFKFB4-IN-1 (0-25  $\mu$ M, 24 h) suppresses PFKFB4 protein levels and suppresses glycolytic metabolism in MCF-7 cells, with markedly reduced intracellular ATP and NADP<sup>+</sup>/NADPH levels<sup>[1]</sup>. 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<sup>[1]</sup>.

### 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.

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