Proteins

Screening Libraries

Product Data Sheet

CYP4Z1-IN-1

Cat. No.: HY-152159 CAS No.: 2760611-38-7 Molecular Formula: $C_{13}H_{18}N_{2}O_{3}$

Molecular Weight: 250.29

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Please store the product under the recommended conditions in the Certificate of Storage:

Analysis.

BIOLOGICAL ACTIVITY

Description CYP4Z1-IN-1 (compound 7c) is a potent CYP4Z1 inhibitor, with an IC₅₀ of 41.8 nM. CYP4Z1-IN-1 decreases the expression of

breast CSCs stemness markers, spheroid formation, and metastatic ability as well as tumor-initiation capability in a

concentration-dependent manner in vitro and in vivo^[1].

IC₅₀ & Target CYP4Z1 CYP4F11 CYP4F12 CYP2D6

> $41.8 \pm 1.4 \text{ nM (IC}_{50})$ 291.3 ± 46 nM (IC₅₀) $1598.3 \pm 5 \text{ nM (IC}_{50})$ >10 000 nM (IC₅₀)

CYP2C9 CYP3A4

>10 000 nM (IC₅₀) >10 000 nM (IC₅₀)

In Vitro CYP4Z1-IN-1 (compound 7c) shows antiproliferative activity against breast CSCs (cancer stem cells), with an IC $_{50}$ of 483 \pm 2.5

CYP4Z1-IN-1 (0.8-51.2 µM, 24 h) suppresses the expression of stemness markers (P-gp, Oct3/4, Nanog, ALDH1A1, and Sox2) in

breast cancer cells^[1].

CYP4Z1-IN-1 (0.8-51.2 μ M, 24-48 h) attenuates the migration and invasion ability of breast cancer cells^[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis^[1]

Cell Line:	MCF-7 and MDA-MB-231 cells
Concentration:	0.8 μΜ, 3.2 μΜ, 12.8 μΜ, 51.2 μΜ
Incubation Time:	24 h
Result:	Significantly suppressed the protein expression of stemness markers (P-gp, Oct3/4, Nanog, ALDH1A1, and Sox2) in MCF-7 cells in a concentration-dependent manner.

In Vivo CYP4Z1-IN-1 (compound 7c) (2000 mg/kg, orally, for 7 days) shows no evident toxicity and body weight loss in mice^[1].

> CYP4Z1-IN-1 (MCF-7 and MDA-MB-231 cells (12.8 µM, 72 h) implanted in the inguinal mammary gland of mice subcutaneously) blocks the tumor-initiating ability of breast cancer cells[1].

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Animal Model:	$Mice^{[1]}$
Dosage:	2000 mg/kg
Administration:	orally, for 7 days
Result:	Showed that compound 7c was rather safe; no evident toxicity and body weight loss were observed.
	(*)
Animal Model:	BALB/c-nude mice (3-4 week old, female) ^[1]
Dosage:	12.8 μΜ
Administration:	MCF-7 and MDA-MB-231 cells were pre-treated with 7c (12.8 μ M) for 72 h and were then implanted in the inguinal mammary gland of mice subcutaneously
Result:	Blocked the tumor-initiating ability of breast cancer cells.

REFERENCES

[1]. Yuan Y, et al. Identification of a Novel Potent CYP4Z1 Inhibitor Attenuating the Stemness of Breast Cancer Cells through Lead Optimization. J Med Chem. 2022 Dec 8;65(23):15749-15769.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

Tel: 609-228-6898

Fax: 609-228-5909

 $\hbox{E-mail: tech@MedChemExpress.com}$

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA