Product Data Sheet

hDHODH-IN-10

Cat. No.: HY-151381

Molecular Formula: C₂,H₁,ClF₂N

Molecular Formula: $C_{21}H_{15}ClF_4N_2O_4$ Molecular Weight: 470.8

Target: Dihydroorotate Dehydrogenase
Pathway: Metabolic Enzyme/Protease

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

Analysis.

BIOLOGICAL ACTIVITY

In Vitro

hDHODH-IN-10 is a selective, potent and orally active hDHODH inhibitor, with an IC₅₀ value of 10.9 nM. hDHODH-IN-10 forms hydrogen bonds with key residues Arg136 and Gln47. hDHODH-IN-10 inhibits the proliferation of cancer cells. hDHODH-IN-10 can be used in the research of cancers, such as AML, colorectal cancer^[1].

IC₅₀ & Target IC50: hDHODH (10.9 nM)^[1].

hDHODH-IN-10 (compound 7d, 1 nM-100 μ M) displays anti-proliferative activities against multiple human cancer cells^[1]. hDHODH-IN-10 (0.0625-0.25 μ M, 24 h) increases the percentage of S-phase cells in Raji and HCT116 cells^[1].

 $\label{eq:mce} \mbox{MCE has not independently confirmed the accuracy of these methods. They are for reference only.}$

Cell Viability Assay^[1]

Cell Line:	U937, HCT116, A375, Kasumi-1 and KG-1 cells
Concentration:	0-10 μM approximately
Incubation Time:	96 h
Result:	Inhibits cell proliferation with IC $_{50}$ values of 0.1-0.8 $\mu\text{M}.$

Cell Cycle Analysis^[1]

Cell Line:	Raji and HCT116 cells
Concentration:	0.0625, 0.125 and 0.25 μM
Incubation Time:	24 h
Result:	Increased the percentage of S-phase cells from 42.8% to 54.2%, 60.6% and 67.1%, respectively.

In Vivo

hDHODH-IN-10 (compound 7d, 30 mg/kg, oral administration) inhibits tumor growth in Raji and HCT116 cells xenograft mice model^[1].

hDHODH-IN-10 (500 mg/kg, oral administration) exhibits a favorable safety profile [1].

 $\label{eq:mce} \mbox{MCE has not independently confirmed the accuracy of these methods. They are for reference only.}$

Animal Model:	Raji and HCT116 cells xenograft mice model ^[1]
Dosage:	30 mg/kg
Administration:	Oral administration
Result:	Showed a tumor growth inhibitory (TGI) rate of 58.3% (Raji model) and 42.1% (HCT116 model).
Animal Model:	BALB/c mice (acute toxicity assay) ^[1]
Dosage:	500 mg/kg
Administration:	Oral administration
Result:	LD ₅₀ is about 500 mg/kg.
	Induced a weak dysfunction of liver.

REFERENCES

[1]. Chungen Li, et al. Discovery of potent human dihydroorotate dehydrogenase inhibitors based on a benzophenone scaffold. European Journal of Medicinal Chemistry, 2022, 243 (5), 114737.

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

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