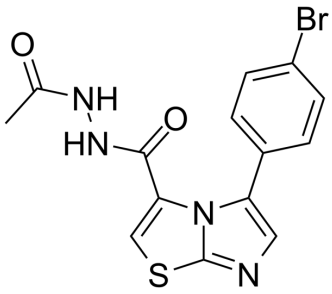
EGFR/HER2/DHFR-IN-1

Cat. No.:	HY-151154
CAS No.:	2820126-37-0
Molecular Formula:	$C_{14}H_{11}BrN_4O_2S$
Molecular Weight:	379.23
Target:	EGFR
Pathway:	JAK/STAT Signaling; Protein Tyrosine Kinase/RTK
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	EGFR/HER2/DHFR-IN-1 is a potent anticancer agent with high selectivity against MCF-7 breast cancer cells. EGFR/HER2/DHFR-IN-1 is a multiple inhibitor of EGFR/HER2 kinase and DHFR, with IC_{50}s of 0.153 μM, 0.108 μM, 0.291 μM, respectively. EGFR/HER2/DHFR-IN-1 arrests cell cycle at G1/S and induces cells apoptosis[1].
IC_{50} & Target	apoptosis; 0.153 μM (EGFR); 0.108 μM (HER2); 0.291 μM (DHFR)[1]

In Vitro

EGFR/HER2-IN-7 (compound 39) shows remarkable broad spectrum cytotoxic potency, with an IC_{50} value of 1.83 μM against MCF-7 breast cancer cell lines[1].

EGFR/HER2-IN-7 (1.83 μM) induces cell apoptosis by arreating cell cycle at G1/S[1].

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

Cell Cycle Analysis[1]

Cell Line:	HepG2 hepatocellular carcinoma, MCF-7 breast cancer, HCT-116 colorectal carcinoma, PC-3 prostate and Hea cervical epithelioid carcinoma
Concentration:	0-1 mM
Incubation Time:	72 hours
Result:	Inhibited EGFR/HER2 kinase and DHFR, while DHFR inhibition caused cell cycle arrest at the S phase while EGFR/HER2 kinase inhibition caused arrest at the G1 phase.

Apoptosis Analysis[1]

Cell Line:	HepG2 hepatocellular carcinoma, MCF-7 breast cancer, HCT-116 colorectal carcinoma, PC-3 prostate and Hea cervical epithelioid carcinoma
Concentration:	0-1 mM
Incubation Time:	72 hours
Result:	Inhibited cancer cells growth and induced apopsosis with IC_{50}s of 3.48 μM (HepG2), 1.83 μM (MCF-7), 6.08 μM (HCT-116), 12.74 μM (PC3), 4.78 μM (Hela), respectively.

In Vivo

Caspase-3 is a lysosomal enzyme involved in apoptosis, and is used as a biomarker for detection of apoptotic cells[1].

EGFR/HER2-IN-7 (compound 39) (10 mg/kg; i.p.; once daily; 20 d) shows anti-breast cancer activity in vivo and increases caspase-3 immunoexpression in brease cancer mice[1].

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Animal Model:	Breast cancer with non-lactating mammary glands animal model in Swiss albino female mice (8-weeks-old)[1]
Dosage:	10 mg/kg
Administration:	Intraperitoneal injection; once daily; 20 days
Result:	Inhibited tumor volume with reduction rate of 76.5%. Reduced body weight with loss rate of 17.4%. Showed the Caspase-3 score of 1.33.

REFERENCES

[1]. Sabry MA, et al. New thiazole-based derivatives as EGFR/HER2 and DHFR inhibitors: Synthesis, molecular modeling simulations and anticancer activity. Eur J Med Chem. 2022 Aug 10;241:114661.

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