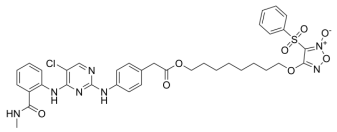
FAK-IN-9

Cat. No.:	HY-149259
CAS No.:	2911655-93-9
Molecular Formula:	$C_{36}H_{38}ClN_7O_8S$
Molecular Weight:	764.25
Target:	FAK
Pathway:	Protein Tyrosine Kinase/RTK
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	FAK-IN-9 (Compound 8f) is a potent and orally active FAK inhibitor with an IC_{50} of 27.44 nM. FAK-IN-9 induces triple-negative breast cancer (TNBC) cell apoptosis[1].
IC_{50} & Target	IC50: 27.44 nM (FAK)[1]

In Vitro

FAK-IN-9 (Compound 8f; 72 h) shows antiproliferative activity with IC_{50}s of 0.167±0.025, 0.126±0.012 and 0.159±0.017 μM against MDA-MB-157, MDA-MB-231 and MDA-MB-453 cells, respectively[1].
FAK-IN-9 (1-4 μM; 72 h) leads to relatively high levels of NO production in a dose-dependent manner in MDA-MB-231 cells[1].
FAK-IN-9 (1-4 μM; 48 h) inhibits invasion and migration of MDA-MB-231 cells[1].
FAK-IN-9 (1-4 μM; 72 h) efficiently blocks FAK mediated-signaling pathways[1].
FAK-IN-9 (4 μM; 72 h) inhibits the formation of focal adhesions (FAs) and stress fibers (SFs) in MDA-MB-231 cells[1].
FAK-IN-9 (1-4 μM; 72 h) induces MDA-MB-231 cell apoptosis[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[1]

Cell Line:	MDA-MB-157, MDA-MB-231, MDA-MB-453 and MCF10A
Concentration:	
Incubation Time:	72 h
Result:	Inhibited proliferation with IC_{50}s of 0.167±0.025, 0.126±0.012, 0.159±0.017 and 2.401±0.131 μM against MDA-MB-157, MDA-MB-231, MDA-MB-453 and MCF10A, respectively.

Cell Invasion Assay[1]

Cell Line:	MDA-MB-231 cells
Concentration:	1, 2 and 4 μM
Incubation Time:	48 h
Result:	The numbers of invasive MDA-MB-231 cells were reduced dose-dependently.

Cell Migration Assay [1]

Cell Line:	MDA-MB-231 cells
Concentration:	1, 2 and 4 μM
Incubation Time:	48 h
Result:	Remarkably block the migration of MDA-MB-231 cells in a dose-dependent manner.

Western Blot Analysis[1]

Cell Line:	MDA-MB-231 cells
Concentration:	1, 2 and 4 μM
Incubation Time:	72 h
Result:	Potently suppressed the autophosphorylation of Y397 in a dose-dependent manner. Decreased the levels of p-AKT, MMP-2 and MMP-9 dose dependently.

Apoptosis Analysis[1]

Cell Line:	MDA-MB-231 cells
Concentration:	1, 2 and 4 μM
Incubation Time:	72 h
Result:	The percentage of apoptotic MDA-MB-231 cells gradually increased ranging from 19.06% to 77.66% at 4 μM.

In Vivo

FAK-IN-9 (Compound 8f; 15 or 30 mg/kg; oral; once daily for 30 days) inhibits MDA-MB-231 lung metastasis in mice[1].

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

Animal Model:	BALB/c nude mice, MDA-MB-231 experimental pulmonary metastasis model[1]
Dosage:	15 or 30 mg/kg
Administration:	Oral, once daily for 30 days
Result:	Potently reduced the numbers of lung tumor nodules dose-dependently.

REFERENCES

[1]. Zhang J, et al. Design, synthesis and evaluation of nitric oxide releasing derivatives of 2,4-diaminopyrimidine as novel FAK inhibitors for intervention of metastatic triple-negative breast cancer. Eur J Med Chem. 2023 Mar 15;250:115192.

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