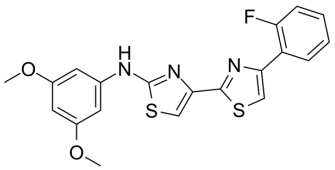
CYP1B1-IN-3

Cat. No.:	HY-152079
CAS No.:	2872575-51-2
Molecular Formula:	$C_{20}H_{16}FN_3O_2S_2$
Molecular Weight:	413.49
Target:	Cytochrome P450
Pathway:	Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	CYP1B1-IN-3 is a potent and selective CYP1B1 inhibitor with IC_{50} values of 6.6, 347.3, >10000 nM for CYP1B1, CYP1A1, CYP1A2, respectively. CYP1B1-IN-3 inhibits cell migration and invasion. CYP1B1-IN-3 inhibits P-gp, AKT/ERK, FAK/SRC, and EMT pathways[1].		
IC_{50} & Target	CYP1B1 6.6 nM (IC_{50})	CYP1A1 347.3 nM (IC_{50})	CYP1A2 >10000 nM (IC_{50})

In Vitro

CYP1B1-IN-3 (compound 77) (3.75-30.0 μM; 72 h) increases the sensitivity of A549/Taxol cells to Taxol (0.06-1 μM)[1].

CYP1B1-IN-3 (2.5, 5, 10 μM) inhibits the cell migration and invasion in DMBA-induced A549 cells that overexpressed CYP1B1 and A549/Taxol cells that overexpressed CYP1B1[1].

CYP1B1-IN-3 (2.5, 5, 10 μM; 24 h) inhibits AKT/ERK, FAK/SRC, and EMT pathways in A549/Taxol cells[1].

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

Western Blot Analysis[1]

Cell Line:	A549/Taxol cells
Concentration:	2.5, 5, 10 μM
Incubation Time:	24 h
Result:	Decreased the expression of P-gp, p-AKT, AKT, p-ERK1/2 (T202/Y204), ERK1/2, p-FAK (Y576), FAK, p-SRC in a dose-dependent manner.

REFERENCES

[1]. Mao J, et al. Structure-Based Drug Design and Synthesis of Novel N-Aryl-2,4-bithiazole-2-amine CYP1B1-Selective Inhibitors in Overcoming Taxol Resistance in A549 Cells. J Med Chem. 2022 Dec 22;65(24):16451-16480.

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

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