Pks13-TE inhibitor 3

Cat. No.: HY-151599

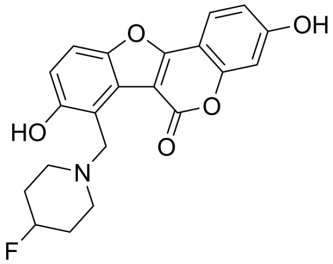
Molecular Formula: $C_{21}H_{18}FNO_5$

Molecular Weight: 383.37

Target: Bacterial

Pathway: Anti-infection

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



BIOLOGICAL ACTIVITY

Description	Pks13-TE inhibitor 3 (compound 23) is a 13-Thioesterase (Pks13-TE) inhibitor (IC_{50}=1.55 μM). Pks13-TE inhibitor 3 shows good anti-tuberculosis activity against both agent-sensitive and drug-resistant Mtb strains (MIC=0.0625-0.25 μg/mL). Pks13-TE inhibitor 3 can be used in studies of multidrug-resistant TB and extensively drug-resistant TB[1].
IC_{50} & Target	IC50: 1.55 μM (Pks13-TE)[1].
In Vitro	Pks13-TE inhibitor 3 (0-5.43 μM; 7 days) demonstrates potent activities against DS (drug-susceptible Mtb strain)-tuberculosis)-TB and DR (drug-resistant strain of Mtb-tuberculosis)-TB strains with MIC range of 0.0625-0.25 μg/mL[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only. Cell Viability Assay[1]

Cell Line:	DS (drug-susceptible Mtb strain)-tuberculosis (V4207), MDR (multidrug-resistant strain of Mtb, resistance to isoniazid and rifampin)-tuberculosis (V2475 and KZN494), XDR (extensively drug-resistant strain of Mtb resistant to isoniazid, rifampin, levofloxacin ofloxacin, and kanamycin)-tuberculosis (TF274 and R506) strains
Concentration:	0-5.43 μM (0-2048 μg/mL)
Incubation Time:	7 days
Result:	Inhibited V4207/DS Mtb strain (MIC=0.125 μg/mL), V2475/MDR (MIC=0.125-0.25 μg/mL), KZN494/MDR (MIC=0.0625-0.125 μg/mL), TF274/XDR (MIC=0.0625 μg/mL) and R506/XDR (MIC=0.0625 μg/mL) Mtb strains.

REFERENCES

[1]. Zhang W, et al. Structure-Based Optimization of Coumestan Derivatives as Polyketide Synthase 13-Thioesterase(Pks13-TE) Inhibitors with Improved hERG Profiles for Mycobacterium tuberculosis Treatment. J Med Chem. 2022 Oct 13;65(19):13240-13252.

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

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