KPC-2-IN-1

Cat. No.: HY-150766

CAS No.: 2232877-85-7

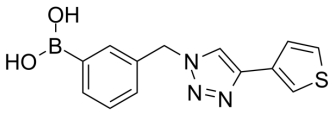
Molecular Formula: $C_{13}H_{12}BN_3O_2S$

Molecular Weight: 285.13

Target: Bacterial

Pathway: Anti-infection

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



BIOLOGICAL ACTIVITY

Description	KPC-2-IN-1, boronic acid derivative, is a potent KPC-2 inhibitor with K_i of 0.032 μM. KPC-2-IN-1 enhances the activity of cefotaxime in KPC-2 expressing E. coli. KPC-2-IN-1 exhibits well tolerated in human HEK-293 cells, which can be used for the study of E. coli resistance to β-lactam antibiotics[1][2].
IC_{50} & Target	Ki: 0.032 μM (KPC-2)[1].
In Vitro	KPC-2-IN-1 (compound 2e) (50 μg/mL; 16 h) enhances the activity of CTX or MEM in KPC-2 expressing E. coli and (5 μg/mL; 16 h) also shows good combination activity of increasing CTX or MEM susceptibility to E. coli NCTC 10418[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only. Cell Viability Assay[1]

Cell Line:	E. coli BL21 DE3 (KPC-2 producing) and NCTC 10418
Concentration:	5, 50 μg/mL (combine with cefotaxime (CTX) or meropenem (MEM)).
Incubation Time:	16 h
Result:	Decreased the MIC of CTX (16 μg/mL) as well as MEM (>64 μg/mL) to ≤ 0.03 or ≤0.06 μg/mL (~512 to >1000-fold increase in susceptibility) against E. coli BL21 DE3 and NCTC 10418.

REFERENCES

[1]. Zhou J, et al. Triazole-substituted phenylboronic acids as tunable lead inhibitors of KPC-2 antibiotic resistance. Eur J Med Chem. 2022 Jun 28;240:114571.

[2]. Zhou J, et al. Boronic acid inhibitors of the class A β-lactamase KPC-2. Bioorg Med Chem. 2018 Jul 15;26(11):2921-2927.

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

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