

Product Data Sheet

Anticancer agent 164

 Cat. No.:
 HY-128634

 CAS No.:
 2235393-30-1

 Molecular Formula:
 C₂₁H₂₃F₃N₈O₂S₂

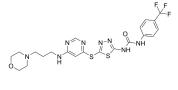
Molecular Weight: 540.58

Target: Apoptosis; PI3K; MEK

Pathway: Apoptosis; PI3K/Akt/mTOR; MAPK/ERK Pathway

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

Analysis.



BIOLOGICAL ACTIVITY

CML-IN-1 (compound 7) is a potent anticancer agent. CML-IN-1 displays very good induced-apoptosis effect for human chronic myeloid leukemia (CML) cell line K562. CML-IN-1 exerts its effect via a significantly reduced protein phosphorylation of PI3K/Akt signal pathway. CML-IN-1 (compound 4) also inhibits cell proliferation by suppressing the MEK/ERK signaling pathway in colorectal cancer^{[1][2]}.

In Vitro CML-IN-1 (compound 7) exhibits the least cellular toxicity and better biological activity in cellular assays (K562, IC₅₀: 0.038 μ _M)^[1]

CML-IN-1 (compound 4) significantly inhibits HCT116 cell proliferation with IC₅₀ values of $8.04 \pm 0.94 \,\mu\text{M}$ after 48 h and $5.52 \pm 0.42 \,\mu\text{M}$ after 72 h, respectively^[2].

CML-IN-1 (compound 4) inhibits colony formation, migration, and invasion of HCT116 cells in a dose-dependent manner, as well as inducing cell apoptosis and arresting the cell cycle in the G2/M phase^[2].

CML-IN-1 (compound 4) inhibits the activation of the MEK/ERK signaling in HCT116 cells^[2].

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

REFERENCES

[1]. Li W, et al. Design and synthesis of novel 1-phenyl-3-(5-(pyrimidin-4-ylthio)-1,3,4-thiadiazol-2-yl)urea derivatives with potent anti-CML activity throughout PI3K/AKT signaling pathway. Bioorg Med Chem Lett. 2019 Jul 15;29(14):1831-1835.

[2]. Li W, et al. A novel 4-(1,3,4-thiadiazole-2-ylthio) pyrimidine derivative inhibits cell proliferation by suppressing the MEK/ERK signaling pathway in colorectal cancer. Acta Pharm. 2023 Sep 14;73(3):489-502.

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

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