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# TH588

产品编号: D50873
CAS: 1609960-31-7
分子式: C13H12Cl2N4
纯度: ≥98%
InChi: InChI=1S/C13H12Cl2N4/c14-9-3-1-2-8(12(9)15)10-6-11(17-7-4-5-7)19-13(16)18-10/h1-3,6-7H,4-5H2,(H3,16,17,18,19)
InChi Key: PNMYJIOQIAEYQL-UHFFFAOYSA-N
Smiles: NC1N=C(C=C(N=1)C1C=CC=C(Cl)C=1Cl)NC1CC1
外观: 固体粉末
作用通路: DNA/RNA Synthesis
溶解性: DMSO up to 50 mM
保存条件: Store in dry, dark place for one year.
产品介绍: TH588 is a novel potent, selective and cell permeable inhibitor of the nudix hydrolase family MTH1 protein with an IC50 of ~5 nM. Protein co-crystal structures demonstrate that TH588 binds in the active site of MTH1. It has excellent selectivity over other nudix family proteins and kinases present in the selectivity panel. The MTH1 protein sanitizes oxidized dNTP pools to prevent incorporation of damaged bases during DNA replication. Although MTH1 is non-essential in normal cells, the cancer cells require MTH1 activity to avoid incorporation of oxidized dNTPs. MTH1 inhibition by TH588 causes incorporation of oxidized dNTPs in cancer cells, leading to DNA damage, cytotoxicity and therapeutic responses in patient-derived mouse xenografts. TH588 is a good chemical tool to exemplify the non-oncogene addiction concept for anticancer treatment and validate MTH1 as a drug target.