
(S)-crizotinib

产品编号: D50871

CAS: 1374356-45-2

分子式: C₂₁H₂₂Cl₂FN₅O

纯度: ≥98%

InChi: InChI=1S/C₂₁H₂₂Cl₂FN₅O/c1-12(19-16(22)2-3-17(24)20(19)23)30-18-8-13(9-27-21(18)25)14-10-28-29(11-14)15-4-6-26-7-5-15/h2-3,8-12,15,26H,4-7H₂,1H₃, (H₂,25,27)/t12-/m0/s1

InChi Key: KTEIFNKAUNYNJU-LBPRGKRZSA-N

Smiles: C[C@H](OC1=CC(=CN=C1N)C1=CN(N=C1)C1CCNCC1)C1C(Cl)=CC=C(F)C=1Cl

外观: 固体粉末

作用通路: Apoptosis

溶解性: DMSO: 42 mg/mL (93.26 mM); EtOH: 22 mg/mL (48.85 mM).

保存条件: Store in dry, dark place for one year.

产品介绍: (S)-Crizotinib is a novel potent, selective and cell permeable MTH1 inhibitor with an IC₅₀ of ~72 nM. MTH1 is a nucleotide pool sanitizing enzyme. (S)-Crizotinib disrupts nucleotide pool homeostasis via MTH1 inhibition and induces an increase in DNA single-strand breaks in cancer cells. In vivo it can effectively suppress tumor growth in colon carcinoma xenograft model by once per day oral dosing. (R)-Crizotinib, which is (R)-enantiomer of the drug, is inactive against MTH1 in vitro. Loss-of-function of MTH1 impaired growth of KRAS tumor cells. (S)-Crizotinib is a useful chemical probe to further validate MTH1 as a promising novel class of anticancer target.