
Bractoppin

产品编号: D58302

CAS: 2290527-07-8

分子式: C₂₅H₂₃FN₄O

纯度: 99.65%

InChi Key: InChIKey=UHDGSNOZRAAGIZ-UHFFFAOYSA-N

Smiles: O=C(N1CCN(CC2=CC=CC=C2F)CC1)C3=CC=C4NC(C5=CC=CC=C5)=NC4=C3

外观: 固体粉末

作用通路: Cell Cycle/Checkpoint; DNA Damage/DNA Repair

作用靶点: DNA/RNA Synthesis

溶解性: DMSO: 25 mg/mL (60.32 mM)

保存条件: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

产品介绍: Bractoppin is a drug-like inhibitor of phosphopeptide recognition by the human BRCA1 tandem (t)BRCT domain (IC₅₀ = 0.074 μM), which selectively inhibits substrate binding with nanomolar potency in vitro. Structure-activity exploration suggests that Bractoppin engages BRCA1 tBRCT residues recognizing pSer in the consensus motif, pSer-Pro-Thr-Phe, plus an abutting hydrophobic pocket that is distinct in structurally related BRCT domains, conferring selectivity.