

Product Name	: Bractoppin
Synonyms	: —
Cat No.	: M24041
CAS Number	: 2290527-07-8
Molecular Formula	: C ₂₅ H ₂₃ FN ₄ O
Formula Weight	: 414.5
Chemical Name	: —
Description	Bractoppin is a drug-like inhibitor of phosphopeptide recognition by the human BRCA1 tandem (t)BRCT domain (IC ₅₀ = 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.
Pathway	: Others
Target	: Other Targets
Receptor	: Others
Solubility	: DMSO:10 mM
SMILES	: <chem>O=C(N1CCN(CC2=CC=CC=C2F)CC1)C3=CC=C4NC(C5=CC=CC=C5)=NC4=C3</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1.Periasamy J, Kurdekar V, Jasti S, et al. Targeting Phosphopeptide Recognition by the Human BRCA1 Tandem BRCT Domain to Interrupt BRCA1-Dependent Signaling[J]. Cell Chemical Biology, 2018:S245194561830076X.