

BAY-805: A chemical probe for USP21

Version 1.0 (21st February 2023)



Web link for more details: <https://www.thesgc.org/chemical-probes/BAY-805>

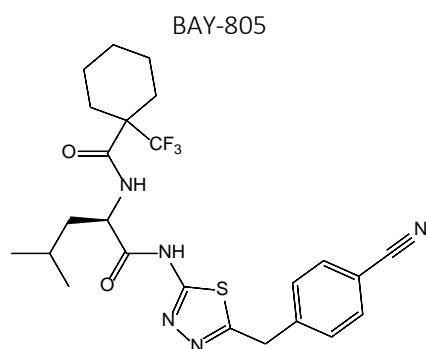
Overview

BAY-805 inhibits USP21 with $IC_{50} < 10$ nM in HTRF and Ub-Rhodamine assays. BAY-728 is a closely related negative control with $IC_{50} > 12$ micromolar.

Summary

Chemical Probe Name	BAY-805
Negative control compound	BAY-728
Target(s) (synonyms)	USP21 (ubiquitin-specific-processing protease 21)
Recommended <i>in vitro</i> assay concentration	≤ 0.1 μ M; use with negative control for best interpretation of data
Suitability for <i>in vivo</i> use and recommended dose	This chemical probe was not tested for <i>in vivo</i> use.
Publications	https://pubs.acs.org/doi/10.1021/acs.jmedchem.2c01933
Orthogonal chemical probes	
<i>In vitro</i> assay(s) used to characterise	HTRF, Ub-Rhodamine, SPR
Cellular assay(s) for target-engagement	CETSA (HiBiT), NF κ B reporter assay
ChemicalProbes.org	

Chemical Probe & Negative Control Structures and Use



SMILES:

CC(C)C[C@H](C(Nc1nnc(Cc2ccc(C#N)cc2)s1)=O)NC(C1(C)C(F)(F)F)=O

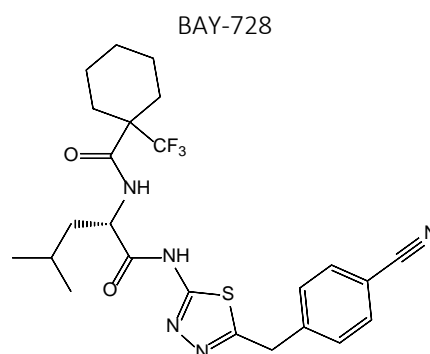
InChiKey: LXRBPWHQMGKMRT-GOSISDBHSA-N

Molecular weight: 507.2

Storage: As a dry powder or as DMSO stock solutions (10 mM) at -20 °C.

DMSO stocks beyond 3-6 months or 2 freeze/thaw cycles should be tested for activity before use

Dissolution: Soluble in DMSO up to 50 mM; use only 1 freeze/thaw cycle per aliquot



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Chemical Probe Profile

In vitro Potency & Selectivity: BAY-805 inhibits USP21 with $IC_{50} = 6$ nM (HTRF).

Potency in Cells and Cellular Target Engagement: HiBiT target engagement $EC_{50} = 95$ nM.