OICR-41103: A chemical probe DCAF1

Version 1.0 (23rd April 2025)

Web link for more details: https://www.thesgc.org/chemical-probes/OICR-41103

Overview

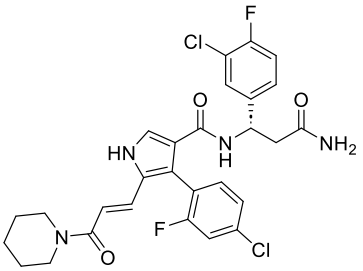
The Structural Genomics Consortium (SGC) in collaboration with the Drug Discovery Program at the Ontario Institute for Cancer Research (OICR) has discovered a chemical probe OICR-41103 for DCAF1 (DDB1-Cul4 associated factor 1).

Summary

Chemical Probe Name	OICR-41103
Negative control compound	OICR-41103N
Target(s) (synonyms)	DCAF1 (VprBP)
Recommended *in vitro* assay concentration	1 µM; use with negative control for best interpretation of data
Suitability for *in* vivo use and recommended dose	This chemical probe was not tested for *in vivo* use.
Publications	
Orthogonal chemical probes	N/A
In vitro assay(s) used to characterise	SPR, DSF, ITC
Cellular assay(s) for target-engagement	NanoBRET, HiBiT CETSA
ChemicalProbes.org	

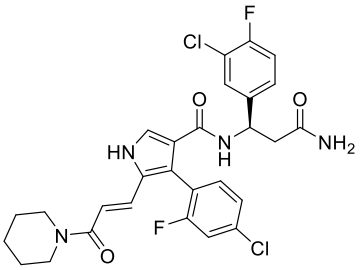
Chemical Probe & Negative Control Structures and Use

OICR-41103



SMILES: O=C(C1=CNC(/C=C/C(N2CCCCC2)=O)=C1C3=C(F)C=C(Cl)C=C3)N[C@H](C4=CC=C(F)C(Cl)=C4)CC(N)=O
InChiKey: WQUCFJCZXPDBNP-KDLSMAQYSA-N
Molecular weight: 575.4
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

OICR-41103N



SMILES: O=C(C1=CNC(/C=C/C(N2CCCCC2)=O)=C1C3=C(F)C=C(Cl)C=C3)N[C@@H](C4=CC=C(F)C(Cl)=C4)CC(N)=O
InChiKey: WQUCFJCZXPDBNP-HCXLOTKHSA-N
Molecular weight: 575.4
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

Chemical Probe Profile

In vitro Potency & Selectivity: In a SPR assay, OICR-41103 binds DCAF1 (WDR) with K_D = 2 nM.

Potency in Cells and Cellular Target Engagement: In an intact cell-based nanoBRET assay, OICR-41103 inhibited the interaction between DCAF1 WDR and a tracer (based on a literature DCAF1 ligand) with EC_{50} = 130 nM.