

OICR11029: A chemical probe for BCL6.

Version 1.0 (28th January 2024)



Web link for more details: <https://www.thesgc.org/chemical-probes/OICR11029>

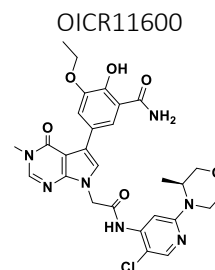
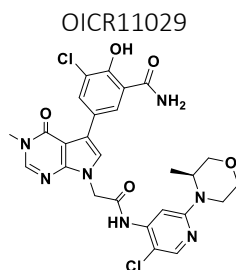
Overview

A collaboration among OICR, University Health Network (in Toronto), and Janssen has developed a chemical probe **OICR11029** for the BTB domain of BCL6.

Summary

Chemical Probe Name	OICR11029
Negative control compound	OICR11600
Target(s) (synonyms)	BCL6
Recommended concentration for cellular use	Use at 1 μ M; recommend to perform a dose-response as different cell lines may require different concentrations. 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://doi.org/10.1021/acsmchemlett.2c00502
Orthogonal chemical probes	
<i>In vitro</i> assay(s) used to characterise	SPR
Cellular assay(s) for target-engagement	cellular luciferase assay in SUDHL4 cells, Karpass-422 (BCL6-dependent) short-term growth inhibition assay

Chemical Probe & Negative Control Structures and Use



SMILES:

CN1C=NC2=C(C1=O)C(C3=CC(C(N)=O)=C(O)C(Cl)=C3)=CN2CC(NC4=C(Cl)C=NC(N5CCOC[C@@H]5C)=C4)=O

InChiKey: NDRFFOKFYGUOKD-ZDUSSCGKSA-N

Molecular weight: 586.4

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

SMILES:

CN1C=NC2=C(C1=O)C(C3=CC(C(N)=O)=C(O)C(OCC)=C3)=CN2CC(NC4=C(Cl)C=NC(N5CCOC[C@@H]5C)=C4)=O

InChiKey: PWMORLQFVWCZTJ-HNNXBMFYSA-N

Molecular weight: 596

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 (cell-free) Potency & Selectivity: OICR11029 binds the BTB domain of BCL6 with $K_D = 10$ nM (SPR).

Potency in Cells and Cellular Target Engagement: OICR11029 displayed an IC_{50} of 375 nM in the cellular luciferase assay in SUDHL4 cells and 602 nM in the Karpass-422 short term growth inhibition assay. NB: Karpass-422 is a BCL6-dependent cancer cell line.