

SGC-UBD253: A chemical probe for HDAC6

Version 2.0 (02nd February 2022)



Web link for more details: <https://www.thesgc.org/chemical-probes/SGC-UBD253>

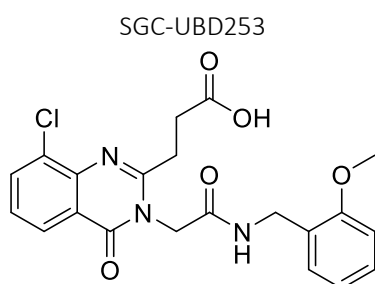
Overview

SGC in collaboration with [Professor Mark Lautens](#) at the University of Toronto has developed the first chemical probe **SGC-UBD253** for the ubiquitin binding domain (UBD) of HDAC6. **SGC-UBD253** binds potently to HDAC6-UBD with $K_D = 84$ nM (SPR). **SGC-UBD253N** is a closely related negative control with $K_D = 32$ micromolar (SPR).

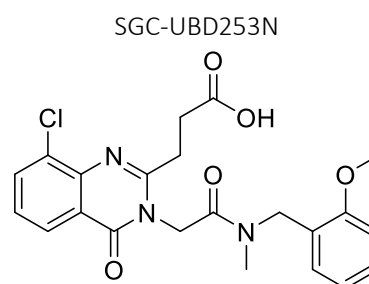
Summary

Chemical Probe Name	SGC-UBD253
Negative control compound	SGC-UBD253N
Target(s) (synonyms)	HDAC6(histone deacetylase 6)
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	_____
Orthogonal chemical probes	
<i>In vitro</i> assay(s) used to characterise	SPR, FP, ITC
Cellular assay(s) for target-engagement	NanoBRET, in cell western
ChemicalProbes.org	

Chemical Probe & Negative Control Structures and Use



SMILES: COc1ccccc1CNC(CN1C(CCC(O)=O)=Nc2c(cccc2[Cl])C1=O)=O
InChiKey: YLHSFRZHEMHKAF-UHFFFAOYSA-N
Molecular weight: 429
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: CN(Cc1ccccc1OC)C(CN1C(CCC(O)=O)=Nc2c(cccc2[Cl])C1=O)=O
InChiKey: KICWUCVHRSAASF-UHFFFAOYSA-N
Molecular weight: 443
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: SGC-UBD253 binds the UBD domain of HDAC6 with $K_D = 84$ nM (SPR).

Potency in Cells and Cellular Target Engagement: NanoBRET measurements showed $EC_{50} = 1.9$ μ M.