

# MRK-952: A chemical probe for NUDT5

Version 1.0 (15<sup>th</sup> October 2022)

Web link for more details: <https://www.thesgc.org/chemical-probes/MRK-952>

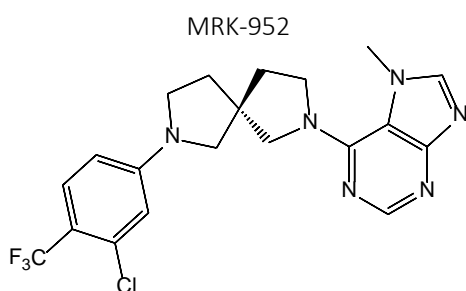
## Overview

**MRK-952** inhibits the hydrolase activity of NUDT5 with  $IC_{50} = 85$  nM. To study the cellular on-target engagement an energy transfer probe (NU074573a) was developed. In the nanoBRET assay MRK-952 inhibited NUDT5 with  $EC_{50} = 23.5 \pm 4$  nM. **MRK-952-NC** is a closely related negative control with  $IC_{50} = 10$  micromolar.

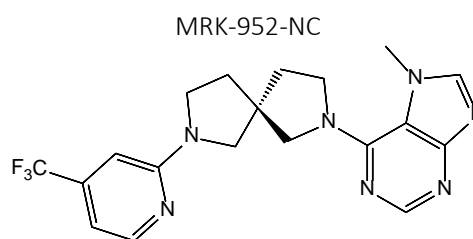
## Summary

Chemical Probe Name	MRK-952
Negative control compound	MRK-952NC
Target(s) (synonyms)	NUDT5
Recommended <i>in vitro</i> assay concentration	$\leq 0.1$ $\mu$ 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	TH5427
<i>In vitro</i> assay(s) used to characterise	AMP Glo
Cellular assay(s) for target-engagement	NanoBRET
ChemicalProbes.org	

## Chemical Probe & Negative Control Structures and Use



SMILES: Cn1cnc2c1c(ncn2)N1CC[C@]2(CCN(C2)c2ccc(c(c2)[Cl])C(F)(F)F)C1  
InChiKey: CAPZLSKZPWSIKV-LQANCHMSA-N  
Molecular weight: 436.1  
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: Cn1cnc2c1c(ncn2)N1CC[C@]2(CCN(C2)c2cc(ccn2)C(F)(F)F)C1  
InChiKey: HSIKTHHVIENBG-SFHVURJKSA-N  
Molecular weight: 403.2  
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

## Chemical Probe Profile

*In vitro* Potency & Selectivity: MRK-952 inhibits the hydrolase activity with  $IC_{50} = 85$  nM .

*Potency in Cells and Cellular Target Engagement:* MRK-952 engages NUDT5 in a nanoBRET assay with an  $EC_{50} = 23.5 \pm 4$  nM.