



Certificate of Analysis

www.tocris.com

Product Name: LCL 161, phenol Catalog No.: 7178 Batch No.: 1

CAS Number: 2095244-42-9

IUPAC Name: tert-Butyl ((S)-1-(((S)-1-cyclohexyl-2-((S)-2-(4-(3-hydroxybenzoyl)thiazol-2-yl)pyrrolidin-1-yl)-2-oxoethyl)amino)-1-

oxopropan-2-yl)(methyl)carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{42}N_4O_6S.\frac{1}{4}H_2O$

Batch Molecular Weight: 603.26

Physical Appearance: White solid

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.72 7.1 9.29 Found 61.38 7.13 9.13

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

Product Information

Print Date: Mar 20th 2023

www.tocris.com

Product Name: LCL 161, phenol Catalog No.: 7178 1

CAS Number: 2095244-42-9

IUPAC Name: tert-Butyl ((S)-1-(((S)-1-cyclohexyl-2-((S)-2-(4-(3-hydroxybenzoyl)thiazol-2-yl)pyrrolidin-1-yl)-2-oxoethyl)amino)-1-

oxopropan-2-yl)(methyl)carbamate

Description:

LCL 161, phenol is a functionalized IAP (XIAP and cIAP) ligand for PROTAC® research and development. Boc protected LCL 161. Supplied with a phenol functional handle for ready conjugation to a linker/target protein ligand. NanoBRET assays show EC50 values of 7.5, 18.2 and 25.3 nM for cIAP1, XIAP and cIAP2 proteins, respectively. Part of a range of functionalized tool molecules for PROTAC R&D. Please contact us for SD files of our available Degrader Building Blocks. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₁H₄₂N₄O₆S.1/4H₂O

Batch Molecular Weight: 603.26 Physical Appearance: White solid

Minimum Purity: ≥95%

Batch Molecular Structure:

Storage: Store at -20°C

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Schwalm et al (2022) A toolbox for the generation of chemical probes for baculovirus IAP repeat containing proteins. Front.Cell.Dev.Biol. **10** 886537. PMID: 35721509.

Ohoka et al (2017) In vivo knockdown of pathogenic proteins via specific and nongenetic inhibitor of apoptosis protein (IAP)-dependent protein erasers (SNIPERs). J.Biol.Chem. **292** 4556. PMID: 28154167.

Shimokawa et al (2017) Targeting the allosteric site of oncoprotein BCR-ABL as an alternative strategy for effective target protein degradation. ACS Med.Chem.Lett. **8** 1042. PMID: 29057048.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use