

**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

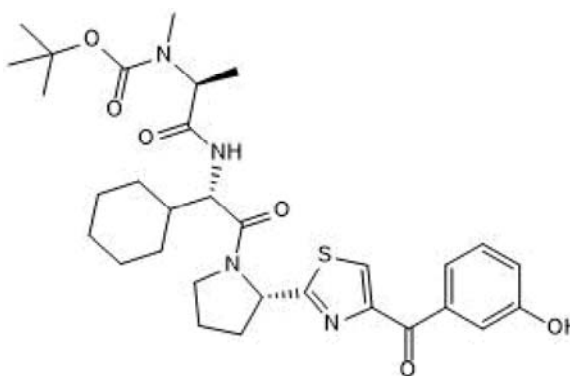
**Batch Molecular Formula:** C<sub>31</sub>H<sub>42</sub>N<sub>4</sub>O<sub>6</sub>S·1/4H<sub>2</sub>O

**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

**<sup>1</sup>H 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

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**Description:**

LCL 161, phenol is a functionalized IAP (XIAP and cIAP) ligand for PROTAC<sup>®</sup> 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 EC<sub>50</sub> 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 Degradator Building Blocks. PROTAC<sup>®</sup> 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:**

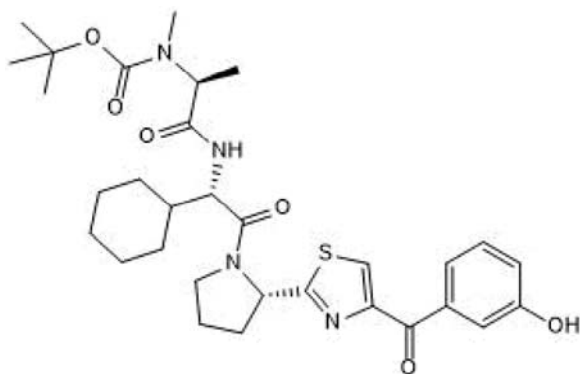
Batch Molecular Formula: C<sub>31</sub>H<sub>42</sub>N<sub>4</sub>O<sub>6</sub>S·½H<sub>2</sub>O

Batch Molecular Weight: 603.26

Physical Appearance: White solid

**Minimum Purity:** ≥95%

**Batch Molecular Structure:**



**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.

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