bio-techne
TOCRIS

Print Date: Mar 20th 2023

Certificate of Analysis

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Product Name: **A 410099.1, amine** **Catalog No.: 6471** **Batch No.: 4**

CAS Number: 2374122-37-7

IUPAC Name: *tert*-Butyl [(*S*)-1-[[(*S*)-2-[(2*S*,4S)-4-amino-2-[[(*R*)-1,2,3,4-tetrahydronaphthalen-1-yl]carbamoyl]pyrrolidin-1-yl]-1-cyclohexyl-2-oxoethyl]amino]-1-oxopropan-2-yl](methyl)carbamate hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

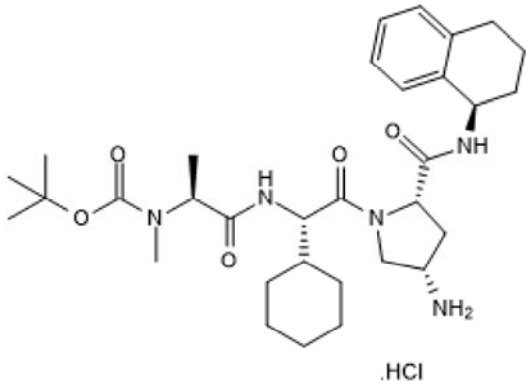
Batch Molecular Formula: $C_{32}H_{49}N_5O_5.HCl.1¼H_2O$

Batch Molecular Weight: 642.74

Physical Appearance: White solid

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.8	8.23	10.9
Found	59.64	8.21	10.88

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

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

A 410099.1, amine is a functionalized IAP ligand for PROTAC® research and development. Boc protected A 410099.1 (Cat.No. 6470). Supplied with an amine functional handle for ready conjugation to a linker/target protein ligand. NanoBRET assays show EC_{50} values of 4.6, 9.2 and 15.6 nM for cIAP1, cIAP2 and XIAP 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:

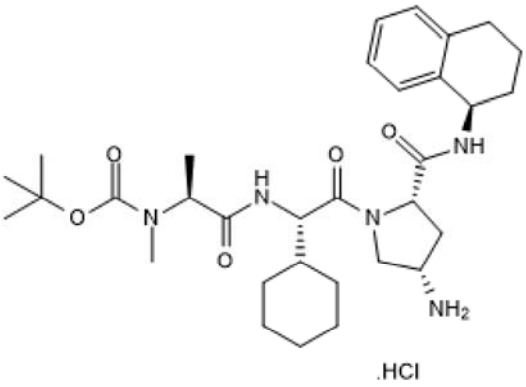
Batch Molecular Formula: $C_{32}H_{49}N_5O_5.HCl.1¼H_2O$

Batch Molecular Weight: 642.74

Physical Appearance: White solid

Minimum Purity: ≥98%

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.

Tinworth *et al* (2019) PROTAC-mediated degradation of Bruton's tyrosine kinase is inhibited by covalent binding. ACS Chem.Biol. ***14*** 342. PMID: 30807093.