TOCRIS
a bio-techne brand

Print Date: Mar 22nd 2021

Certificate of Analysis

www.tocris.com

Product Name: **A 410099.1 amide-PEG5-amine** **Catalog No.: 7221** **Batch No.: 1**

CAS Number: 2446474-11-7

IUPAC Name: *tert*-Butyl ((*S*)-1-(((*S*)-2-((2*S*,4*S*)-4-(17-amino-3,6,9,12,15-pentaoxaheptadecanamido)-2-(((*R*)-1,2,3,4-tetrahydronaphthalen-1-yl)carbamoyl)pyrrolidin-1-yl)-1-cyclohexyl-2-oxoethyl)amino)-1-oxopropan-2-yl)(methyl)carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

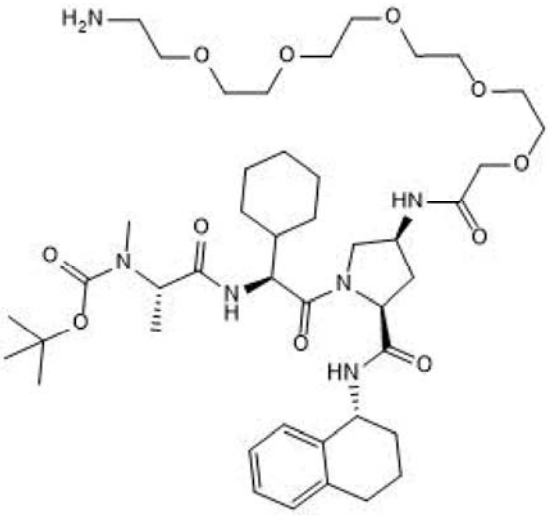
Batch Molecular Formula: $C_{44}H_{72}N_6O_{11}$

Batch Molecular Weight: 861.09

Physical Appearance: White solid

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.37	8.43	9.76
Found	61.47	8.26	9.95

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

Product Name: **A 410099.1 amide-PEG5-amine** **Catalog No.: 7221** **Batch No.: 1**

CAS Number: 2446474-11-7

IUPAC Name: *tert*-Butyl ((*S*)-1-(((*S*)-2-((2*S*,4*S*)-4-(17-amino-3,6,9,12,15-pentaoxaheptadecanamido)-2-(((*R*)-1,2,3,4-tetrahydronaphthalen-1-yl)carbamoyl)pyrrolidin-1-yl)-1-cyclohexyl-2-oxoethyl)amino)-1-oxopropan-2-yl)(methyl)carbamate

Description:

Functionalized IAP ligand for PROTAC® research and development; incorporates an IAP ligand plus an amide-PEG5 linker with terminal amine ready for conjugation to a target protein ligand. Part of a range of functionalized tool molecules for PROTAC R&D. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

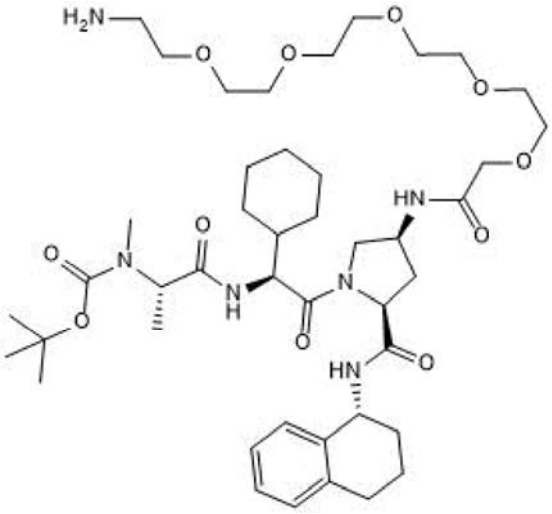
Batch Molecular Formula: $C_{44}H_{72}N_6O_{11}$

Batch Molecular Weight: 861.09

Physical Appearance: White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

Standard retail vials are prepared by lyophilisation. The product may appear as a solid, a gel or a film. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

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