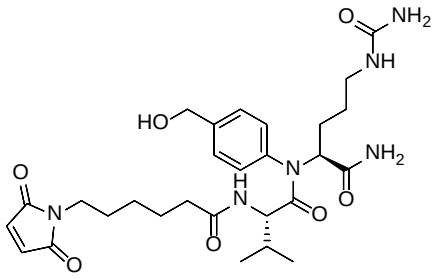
Product data sheet

MedKoo Cat#: 555776 Name: Mc-Val-Cit-PAB CAS: 159857-80-4 (MC-Val-Cit-PAB) Chemical Formula: $C_{28}H_{40}N_6O_7$ Exact Mass: 572.2958 Molecular Weight: 572.663	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Mc-Val-Cit-PAB is a peptide linker molecule used in the synthesis of antibody-drug conjugates (ADCs). It contains a maleimidocaproyl (Mc) group that can be conjugated to an antibody and a p-aminobenzyl (PAB) spacer that allows the peptide to be linked to active compounds, such as anticancer agents. Mc-Val-Cit-PAB is cleaved in vivo by cathepsin B, a protease highly expressed in cancer cells, which confers specificity of the ADC to cancer cells.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	145.0	253.20

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.75 mL	8.73 mL	17.46 mL
5 mM	0.35 mL	1.75 mL	3.49 mL
10 mM	0.17 mL	0.87 mL	1.75 mL
50 mM	0.04 mL	0.17 mL	0.35 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Dubowchik GM, Firestone RA, Padilla L, Willner D, Hofstead SJ, Mosure K, Knipe JO, Lasch SJ, Trail PA. Cathepsin B-labile dipeptide linkers for lysosomal release of doxorubicin from internalizing immunoconjugates: model studies of enzymatic drug release and antigen-specific in vitro anticancer activity. Bioconjug Chem. 2002 Jul-Aug;13(4):855-69. doi: 10.1021/bc025536j. PMID: 12121142.

In vivo study

1. Mondal D, Ford J, Pinney KG. Improved Methodology for the Synthesis of a Cathepsin B Cleavable Dipeptide Linker, Widely Used in Antibody-Drug Conjugate Research. Tetrahedron Lett. 2018 Oct 3;59(40):3594-3599. doi: 10.1016/j.tetlet.2018.08.021. Epub 2018 Aug 14. PMID: 31156276; PMCID: PMC6541422.

7. Bioactivity
Biological target:

MC-Val-Cit-PAB is a cathepsin cleavable ADC linker that is used for making antibody-drug conjugate.

In vitro activity

Product data sheet

A self-immolative p-aminobenzyloxycarbonyl (PABC) spacer between the dipeptides and the DOX was required for rapid and quantitative generation of free drug. DOX release from model substrate Z-Phe-Lys-PABC-DOX 49 was 30-fold faster than from Z-Val-Cit-PABC-DOX 42 with the cysteine protease cathepsin B alone.

Reference: Bioconjug Chem. 2002 Jul-Aug;13(4):855-69. https://pubmed.ncbi.nlm.nih.gov/12121142/

In vivo activity

The Mc-Val-Cit-PABOH linker (1, Fig. 2) displays high plasma stability (half-lives in mice and monkey of 6.0 and 9.6 days, respectively), and has been found to be superior over chemically labile linkers.

Reference: Tetrahedron Lett. 2018 Oct 3;59(40):3594-3599. https://pubmed.ncbi.nlm.nih.gov/31156276/