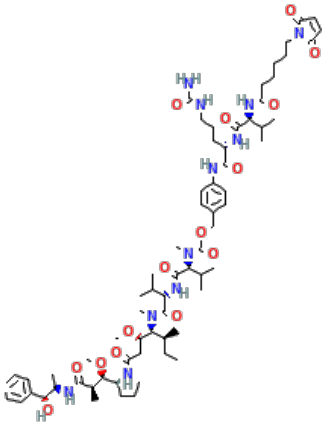
CD BioGlyco
SUITE 201, 17 Ramsey Road, Shirley, NY 11967, USA
Tel: 1-631-637-6119 | Email: info@bioglyco.com

Product Information

Microtubule/Tubulin inhibitor, VcMMAE, Purity ≥98%



Cat. No.: X24-08-YM234

Size: 1 mg; 2 mg; 5 mg; 10 mg

MDL: MFCD25372036

CAS Number: 646502-53-6

Compound CID: 46944733

Synonym: 646502-53-6; Vedotin; MC-Val-Cit-PAB-MMAE; VcMMAE (GMP); [4-[[(2*S*)-5-(Carbamoylamino)-2-[[(2*S*)-2-[6-(2,5-dioxopyrrol-1-yl)hexanoylamino]-3-methylbutanoyl]amino]pentanoyl]amino]phenyl]methyl *N*-[(2*S*)-1-[[(2*S*)-1-[[(3*R*,4*S*,5*S*)-1-[(2*S*)-2-[(1*R*,2*R*)-3-[[(1*S*,2*R*)-1-hydroxy-1-phenylpropan-2-yl]amino]-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl]-3-methoxy-5-methyl-1-oxoheptan-4-yl]-methylamino]-3-methyl-1-oxobutan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]-*N*-methylcarbamate

This product is for research use only and is not intended for diagnostic use.

Product Information

Description	VcMMAE, soluble in DMSO and ethanol and insoluble in water, is an effective cytoskeleton inhibitor, that has the ability to prevent the pathway of cytoskeletal signaling by inhibiting microtubule/tubulin.
Molecular Weight	1316.63
Molecular Formula	$C_{68}H_{105}N_{11}O_{15}$
IUPAC Name	[4-[[(2*S*)-5-(Carbamoylamino)-2-[[(2*S*)-2-[6-(2,5-dioxopyrrol-1-yl)hexanoylamino]-3-methylbutanoyl]amino]pentanoyl]amino]phenyl]methyl *N*-[(2*S*)-1-[[(2*S*)-1-[[(3*R*,4*S*,5*S*)-1-[(2*S*)-2-[(1*R*,2*R*)-3-[[(1*S*,2*R*)-1-hydroxy-1-phenylpropan-2-yl]amino]-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl]-3-methoxy-5-methyl-1-oxoheptan-4-yl]-methylamino]-3-methyl-1-oxobutan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]-*N*-methylcarbamate
InChI	InChI=1S/C68H105N11O15/c1-15-43(8)59(51(92-13)38-55(83)78-37-23-27-50(78)61(93-14)44(9)62(85)71-45(10)60(84)47-24-18-16-19-25-47)76(11)66(89)57(41(4)5)75-65(88)58(42(6)7)77(12)68(91)94-39-46-29-31-48(32-30-46)72-63(86)49(26-22-35-70-67(69)90)73-64(87)56(40(2)3)74-52(80)28-20-17-21-36-79-53(81)33-34-54(79)82/h16,18-19,24-25,29-34,40-45,49-51,56-61,84H,15,17,20-23,26-28,35-39H2,1-14H3,(H,71,85)(H,72,86)(H,73,87)(H,74,80)(H,75,88)(H3,69,70,90)/t43-,44+,45+,49-,50-,51+,56-,57-,58-,59-,60+,61+/m0/s1
InChI Key	NLMBVBUNULOTNS-HOKPPMCLSA-N

© CD BioGlyco. All Rights Reserved.

CD BioGlyco
SUITE 201, 17 Ramsey Road, Shirley, NY 11967, USA
Tel: 1-631-637-6119 | Email: info@bioglyco.com

Canonical SMILES	CCC(C)C(C(CC(=O)N1CCCC1C(C(C)C(=O)NC(C)C(C2=CC=CC=C2)O)OC)OC)N(C)C(=O)C(C(C)C)NC(=O)C(C(C)C)N(C)C(=O)OCC3=CC=C(C=C3)NC(=O)C(CCCNC(=O)N)NC(=O)C(C(C)C)NC(=O)CCCCCN4C(=O)C=CC4=O
Isomeric SMILES	CC[C@H](C)[C@@H]([C@@H](CC(=O)N1CCC[C@H]1[C@@H]([C@@H](C)C(=O)N[C@H](C)[C@H](C2=CC=CC=C2)O)OC)OC)N(C)C(=O)[C@H](C(C)C)NC(=O)[C@H](C(C)C)N(C)C(=O)OCC3=CC=C(C=C3)NC(=O)[C@H](CCCNC(=O)N)NC(=O)[C@H](C(C)C)NC(=O)CCCCCN4C(=O)C=CC4=O
Form	Lyophilized powder
Purity	≥98%
Titer	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects
Solubility	*In vitro*: DMSO: 92 mg/mL (69.87 mM); Water: insoluble; Ethanol: 92 mg/mL (69.87 mM)
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	VcMMAE is a cytoskeletal signaling inhibitor that can be used for its membrane permeability.
Storage	Store at -20ºC, and keep desiccated.

© CD BioGlyco. All Rights Reserved.