

Product Information

Motixafortide

Cat. No.: X23-12-YM1463

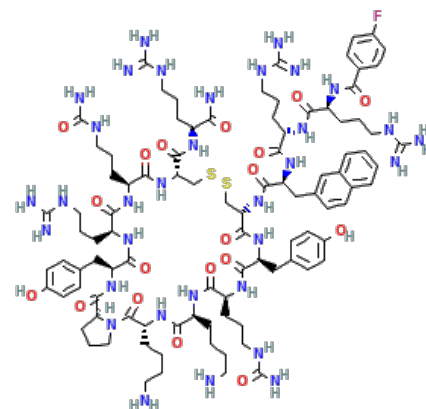
Size: 1 mg; 5 mg; 10 mg; 50 mg

CAS Number: 664334-36-5

Compound CID: 16131686

Synonym: 664334-36-5; BKT140

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



Product Information

Description	Motixafortide inhibits autophagy, through multiple signaling pathways.
Molecular Weight	2159.52
Molecular Formula	C ₉₇ H ₁₄₄ FN ₃₃ O ₁₉ S ₂
IUPAC Name	(3 <i>R</i> ,6 <i>S</i> ,9 <i>S</i> ,12 <i>S</i> ,15 <i>R</i> ,20 <i>R</i> ,23 <i>S</i> ,26 <i>S</i> ,29 <i>S</i> ,32 <i>S</i>)-3,6-Bis(4-aminobutyl)- <i>N</i> -[(2 <i>S</i>)]-1-amino-5-carbamimidamido-1-oxopentan-2-yl]-15-[[(2 <i>S</i>)-2-[[[(2 <i>S</i>)-5-carbamimidamido-2-[[[(2 <i>S</i>)-5-carbamimidamido-2-[[[4-(4-fluorobenzoyl)amino]pentanoyl]amino]pentanoyl]amino]-3-naphthalen-2-ylpropanoyl]amino]-26-(3-carbamimidamidopropyl)-9,23-bis[3-(carbamoylamino)propyl]-12,29-bis[(4-hydroxyphenyl)methyl]-2,5,8,11,14,22,25,28,31-nonaoxo-17,18-dithia-1,4,7,10,13,21,24,27,30-nona-zabicyclo[30.3.0]pentatriacontane-20-carboxamide]
InChI	InChI=1S/C97H144FN33O19S2/c98-60-33-31-58(32-34-60)78(135)119-65(19-8-42-113-93(104)105)79(136)121-68(21-10-44-115-95(108)109)83(140)126-73(51-56-25-30-57-14-1-2-15-59(57)48-56)87(144)130-75-53-152-151-52-74(88(145)118-63(77(101)134)18-7-41-112-92(102)103)129-84(141)69(23-12-46-117-97(111)150)122-81(138)66(20-9-43-114-94(106)107)124-86(143)72(50-55-28-37-62(133)38-29-55)128-90(147)76-24-13-47-131(76)91(148)70(17-4-6-40-100)125-82(139)64(16-3-5-39-99)120-80(137)67(22-11-45-116-96(110)149)123-85(142)71(127-89(75)146)49-54-26-35-61(132)36-27-54/h1-2,14-15,25-38,48,63-76,132-133H,3-13,16-24,39-47,49-53,99-100H2,(H2,101,134)(H,118,145)(H,119,135)(H,120,137)(H,121,136)(H,122,138)(H,123,142)(H,124,143)(H,125,139)(H,126,140)(H,127,146)(H,128,147)(H,129,141)(H,130,144)(H4,102,103,112)(H4,104,105,113)(H4,106,107,114)(H4,108,109,115)(H3,110,116,149)(H3,111,117,150)/t63-,64-,65-,66-,67-,68-,69-,70+,71-,72-,73-,74-,75-,76-/m0/s1
InChI Key	JJVZSYKFCOBILL-KZGZZEQFSA-N
Canonical SMILES	C1CC2C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(CSSCC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)



=O)N2C1)CCCCN)CCCCN)CCCNC(=O)N)CC3=CC=C(C=C3)O)NC(=O)C(CC4=CC5=CC=CC=C5C=C4)NC(=O)C(CCCNC(=N)N)NC(=O)C(CCCNC(=N)N)NC(=O)C6=CC=C(C=C6)F)C(=O)NC(CCCNC(=N)N)C(=O)N)CCCNC(=O)N)CCCNC(=N)N)CC7=CC=C(C=C7)O

Isomeric SMILES

C1C[C@H]2C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](CSSC[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N2C1)CCCCN)CCCCN)CCCNC(=O)N)CC3=CC=C(C=C3)O)NC(=O)[C@H](CC4=CC5=CC=CC=C5C=C4)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCNC(=N)N)NC(=O)C6=CC=C(C=C6)F)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N)CCCNC(=O)N)CCCNC(=N)N)CC7=CC=C(C=C7)O

Form Lyophilized powder

Purity >98%

Stability The product is stable for three years when stored at the recommended temperature in lyophilized powder.

Applications Motixafortide can be studied for its effect on disrupting the interaction between cancer cells and the protective microenvironment of the bone marrow.

Storage Store at -20°C, and keep desiccated.