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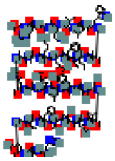
COMPOUND SUMMARY

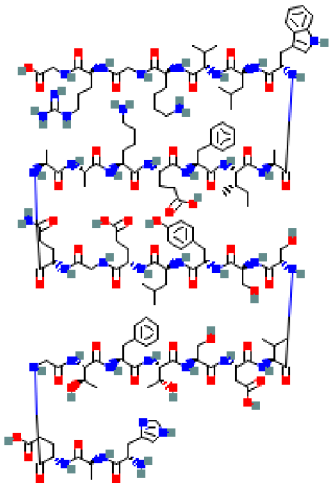
Glucagon-like Peptide-1 (7-37)

PubChem CID	16133830
Structure	 2D Find Similar Structures
Molecular Formula	$C_{151}H_{228}N_{40}O_{47}$
Synonyms	CID 16133830 GLP-1 (7-37) peptide GLP-1 (7-37) human DTXSID50147676 Glucagon-like Peptide-1 (7-37) More...
Molecular Weight	3355.7
Dates	Modify 2023-02-25 Create 2007-07-04

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Status

Conformer generation is disallowed since too many atoms, too flexible

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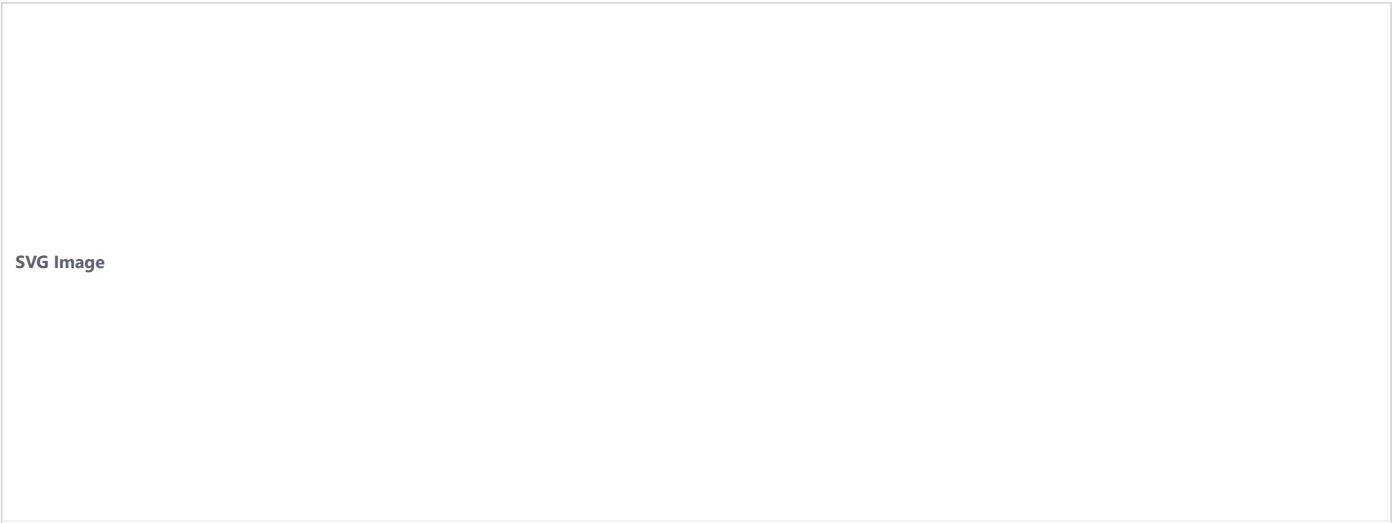
2 Biologic Description

SVG Image	
IUPAC Condensed	H-His-Ala-Glu-Gly-Thr-Phe-Thr-Ser-Asp-Val-Ser-Ser-Tyr-Leu-Glu-Gly-Gln-Ala-Ala-Lys-Glu-Phe-Ile-Ala-Trp-Leu-Val-Lys-Gly-Arg-Gly-OH
Sequence	HAEGTFTSDVSSYLEGQAAKEFIAWLVKGRG
PLN	H-HAEGTFTSDVSSYLEGQAAKEFIAWLVKGRG-OH
HELM	PEPTIDE1{H.A.E.G.T.F.T.S.D.V.S.S.Y.L.E.G.Q.A.A.K.E.F.I.A.W.L.V.K.G.R.G}$$$$
IUPAC	L-histidyl-L-alanyl-L-alpha-glutamyl-glycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L-alpha-aspartyl-L-valyl-L-seryl-L-seryl-L-tyrosyl-L-leucyl-L-alpha-glutamyl-glycyl-L-glutaminyl-L-alanyl-L-alanyl-L-lysyl-L-alpha-glutamyl-L-phenylalanyl-L-isoleucyl-L-alanyl-L-tryptophyl-L-leucyl-L-valyl-L-lysyl-glycyl-L-arginyl-glycine

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3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(4*S*)-5-[[2-[[(2*S*,3*R*)-1-[[(2*S*)-1-[[(2*S*,3*R*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[2-[[(2*S*)-5-amino-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-6-amino-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*,3*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-1-[[(2*S*)-6-amino-1-[[2-[[(2*S*)-5-carbamimidamido-1-(carboxymethylamino)-1-oxopentan-2-yl]amino]-2-oxoethyl]amino]-1-oxohexan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]amino]-4-methyl-1-oxopentan-2-yl]amino]-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl]amino]-1-oxopropan-2-yl]amino]-3-methyl-1-oxopentan-2-yl]amino]-1-oxo-3-phenylpropan-2-yl]amino]-4-carboxy-1-oxobutan-2-yl]amino]-1-oxohexan-2-yl]amino]-1-oxopropan-2-yl]amino]-1-oxopropan-2-yl]amino]-1,5-dioxopentan-2-yl]amino]-2-oxoethyl]amino]-4-carboxy-1-oxobutan-2-yl]amino]-4-methyl-1-oxopentan-2-yl]amino]-3-(4-hydroxyphenyl)-1-oxopropan-2-yl]amino]-3-hydroxy-1-oxopropan-2-yl]amino]-3-hydroxy-1-oxopropan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]amino]-3-carboxy-1-oxopropan-2-yl]amino]-3-hydroxy-1-oxopropan-2-yl]amino]-3-hydroxy-1-oxobutan-2-yl]amino]-1-oxo-3-phenylpropan-2-yl]amino]-3-hydroxy-1-oxobutan-2-yl]amino]-2-oxoethyl]amino]-4-[[(2*S*)-2-[[(2*S*)-2-amino-3-(1*H*-imidazol-4-yl)propanoyl]amino]propanoyl]amino]-5-oxopentanoic acid

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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3.1.2 InChI

InChI=1S/C151H228N40O47/c1-17-77(10)121(148(236)169-81(14)127(215)177-105(60-87-63-160-92-36-25-24-35-90(87)92)138(226)179-101(56-74(4)5)139(227)188-119(75(6)7)146(234)176-94(37-26-28-52-152)130(218)161-65-111(199)170-93(39-30-54-159-151(156)157)129(217)164-68-118(210)211)190-140(228)103(57-84-31-20-18-21-32-84)180-135(223)99(47-51-116(206)207)175-134(222)95(38-27-29-53-153)172-125(213)79(12)166-124(212)78(11)168-133(221)98(44-48-110(155)198)171-112(200)66-162-132(220)97(46-50-115(204)205)174-136(224)100(55-73(2)3)178-137(225)102(59-86-40-42-89(197)43-41-86)181-143(231)107(69-192)184-145(233)109(71-194)185-147(235)120(76(8)9)189-142(230)106(62-117(208)209)182-144(232)108(70-193)186-150(238)123(83(16)196)191-141(229)104(58-85-33-22-19-23-34-85)183-149(237)122(82(15)195)187-113(201)67-163-131(219)96(45-49-114(202)203)173-126(214)80(13)167-128(216)91(154)61-88-64-158-72-165-88/h18-25,31-36,40-43,63-64,72-83,91,93-109,119-123,160,192-197H,17,26-30,37-39,44-62,65-71,152-154H2,1-16H3,(H2,155,198)(H,158,165)(H,161,218)(H,162,220)(H,163,219)(H,164,217)(H,166,212)(H,167,216)(H,168,221)(H,169,236)(H,170,199)(H,171,200)(H,172,213)(H,173,214)(H,174,224)(H,175,222)(H,176,234)(H,177,215)(H,178,225)(H,179,226)(H,180,223)(H,181,231)(H,182,232)(H,183,237)(H,184,233)(H,185,235)(H,186,238)(H,187,201)(H,188,227)(H,189,230)(H,190,228)(H,191,229)(H,202,203)(H,204,205)(H,206,207)(H,208,209)(H,210,211)
(H4,156,157,159)/t77-,78-,79-,80-,81-,82+,83+,91-,93-,94-,95-,96-,97-,98-,99-,100-,101-,102-,103-,104-,105-,106-,107-,108-,109-,119-,120-,121-,122-,123-/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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3.1.3 InChIKey

GCYXWQUSHADNBF-AAEALURTSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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3.1.4 Canonical SMILES

CCC(C)C(C(=O)NC(C)C(=O)NC(CC1=CNC2=CC=CC=C21)C(=O)NC(CC(C)C)C(=O)NC(C(C)C)C(=O)NC(CCCCN)C(=O)NCC(=O)NC(CCCNC(=N)N)C(=O)NCC(=O)NC(=O)C(CC3=CC=CC=C3)NC(=O)C(CCC(=O)O)NC(=O)C(CCCCN)NC(=O)C(C)NC(=O)C(C)NC(=O)C(CCC(=O)N)NC(=O)CNC(=O)C(CCC(=O)O)NC(=O)C(CC(C)C)NC(=O)C(CC4=CC=C(C=C4)O)NC(=O)C(CO)NC(=O)C(CO)NC(=O)C(C(C)C)NC(=O)C(CC(=O)O)NC(=O)C(CO)NC(=O)C(C(C)C)O)NC(=O)C(CC5=CC=CC=C5)NC(=O)C(C(C)O)NC(=O)CNC(=O)C(CCC(=O)O)NC(=O)C(C)NC(=O)C(CC6=CNC=N6)N

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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3.1.5 Isomeric SMILES

CC[C@H](C)[C@@H](C(=O)N[C@@H](C)C(=O)N[C@@H](CC1=CNC2=CC=CC=C21)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CCCCN)C(=O)NCC(=O)N[C@@H](CCCNC(=N)N)C(=O)NCC(=O)O)NC(=O)[C@H](CC3=CC=CC=C3)NC(=O)[C@H](CCC(=O)O)NC(=O)[C@H](CCCCN)NC(=O)[C@H](C)NC(=O)[C@H](C)NC(=O)[C@H](CCC(=O)N)NC(=O)CNC(=O)[C@H](CCC(=O)O)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CC4=CC=C(C=C4)O)NC(=O)[C@H](CO)NC(=O)[C@H](CO)NC(=O)[C@H](C(C)C)NC(=O)[C@H](CC(=O)O)NC(=O)[C@H](CO)NC(=O)[C@H]([C@@H](C)O)NC(=O)[C@H]

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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3.2 Molecular Formula

C151H228N40O47

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3.3 Other Identifiers

3.3.1 CAS

106612-94-6

EPA DSSTox

3.3.2 DSSTox Substance ID

DTXSID50147676

EPA DSSTox

3.4 Synonyms

3.4.1 MeSH Entry Terms

GLP-1 (7-37)
GLP-1(7-37)
GLP-I (7-37)
glucagon-like peptide 1 (7-37)
glucagon-like peptide I (7-37)
glucagon-like-peptide-1 (7-37)
tGLP-1

Medical Subject Headings (MeSH)

3.4.2 Depositor-Supplied Synonyms

CID 16133830
GLP-1 (7-37) peptide
GLP-1 (7-37) human
DTXSID50147676
Glucagon-like Peptide-1 (7-37)
AKOS025142102
1450806-98-0
GLP-1 (7-37)
Glucagon like peptide 1 fragment 7-37 (human)
GLP-1(7-37) acetate(106612-94-6 free base)
Glucagon-Like Peptide 1 Fragment 7-37 human, >=96% (HPLC)
H-HIS-ALA-GLU-GLY-THR-PHE-THR-SER-ASP-VAL-SER-SER-TYR-LEU-GLU-GLY-GLN-ALA-ALA-LYS-GLU-PHE-ILE-ALA-TRP-LEU-VAL-LYS-GLY-ARG-GLY-OH

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