Human microbiome derived synthetic antimicrobial peptides with activity against Gram-negative, Gram-positive, and antibiotic resistant bacteria

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Table of Contents

Predicted secondary structure and data of peptides

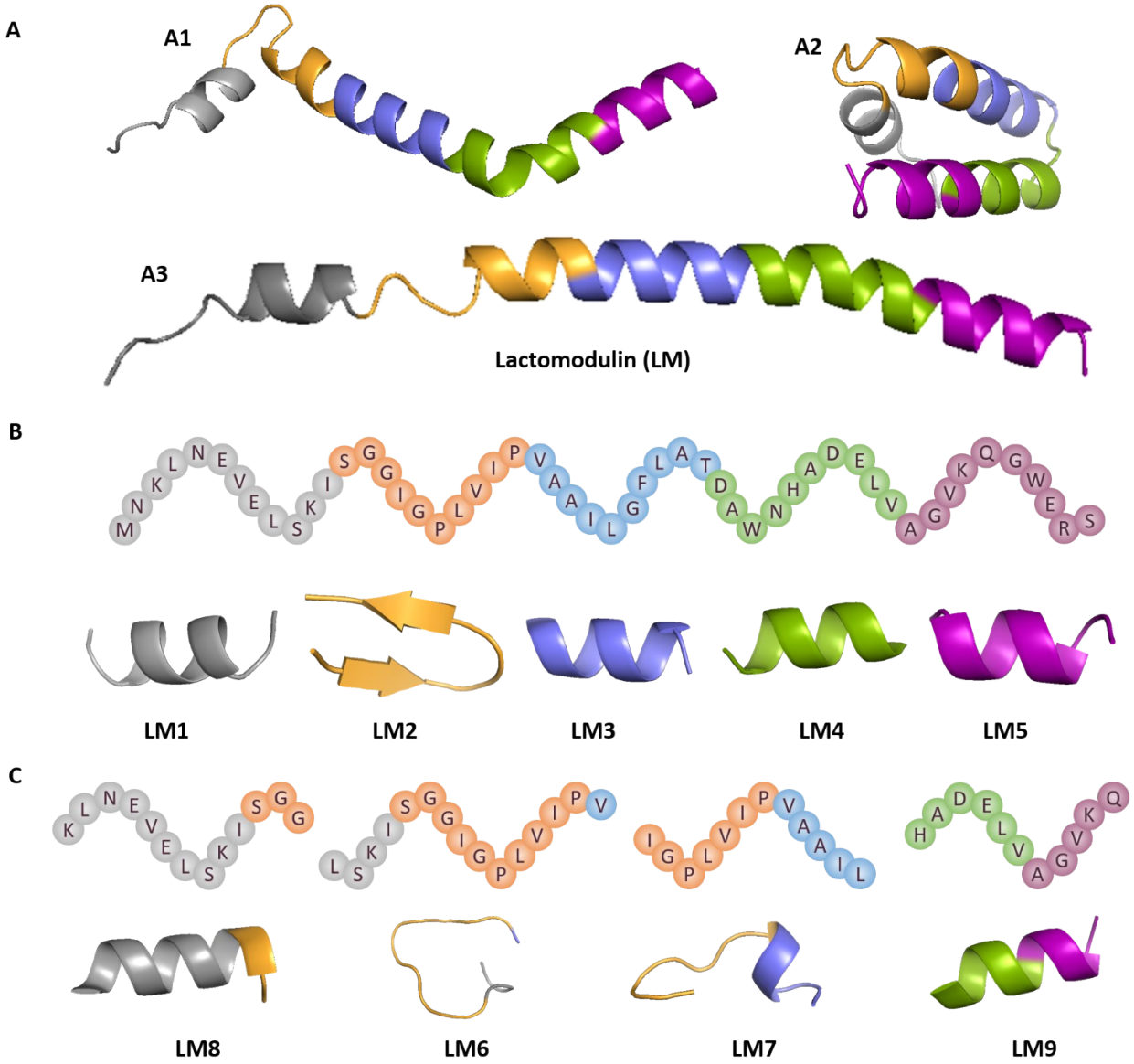


Figure S1. A) Helical structure of lactomodulin as predicted by RoseTTA (A1), Quark (A2), and AlphaFold (A3); B) Amino acid sequence of lactomodulin split into five color-coded peptides LM1-LM5 (grey, orange, blue, green, and purple, respectively) and their structural prediction by PEP-FOLD3; C) Sequence of peptides LM6-LM9 obtained based on AMP prediction using CAMPr3 and their structural prediction by PEP-FOLD3.

Table S1. Novel Lactomodulin derivatives

No.	Sequence	Molecular formula	MW (g/mol)	m/z calcd $[M+H]^+$	m/z found $[M+H]^+$	Δm (ppm)	Yield (%)	Purity (%)
LM1	MNKLNEVELSKI-NH_2	$C_{61}H_{109}N_{17}O_{19}S$	1416.78	1416.7879	1416.7736	10.0933	15.1	76
LM2	SGGIGPLVIP-NH_2	$C_{42}H_{73}N_{11}O_{11}$	908.18	908.5564	908.5530	3.7422	24.0	99
LM3	VAAILGFLAT-NH_2	$C_{47}H_{79}N_{11}O_{11}$	974.27	974.6033	974.6000	3.3860	29.3	96
LM4	DAWNHADELV-NH_2	$C_{51}H_{73}N_{15}O_{17}$	1168.28	1168.5382	1168.5320	5.3058	19.7	97
LM5	AGVKQGWERS-NH_2	$C_{48}H_{77}N_{17}O_{14}$	1116.23	1116.5909	1116.5795	10.2096	19.4	99
LM6	LSKISGGIGPLVIPV-NH_2	$C_{68}H_{121}N_{17}O_{17}$	1448.92	1448.9199	1448.9039	11.0427	10.8	98
LM7	IGPLVIPVAAIL-NH_2	$C_{58}H_{103}N_{13}O_{12}$	1174.62	1174.7922	1174.7838	7.1502	19.5	97
LM8	KLNEVELSKISGG-NH_2	$C_{59}H_{105}N_{17}O_{20}$	1372.67	1372.7774	1372.7755	1.3841	12.5	98
LM9	HADELVAGVKQ-NH_2	$C_{50}H_{84}N_{16}O_{16}$	1165.38	1165.6324	1165.6274	4.2895	14.4	95
LM10	LSKISGGIGP-NH_2	$C_{41}H_{74}N_{12}O_{12}$	927.18	927.5622	927.5567	5.9295	31.6	96
LM11	KISGGIGPLV-NH_2	$C_{43}H_{78}N_{12}O_{11}$	939.24	939.5986	939.5935	5.4278	23.5	97
LM12	LSKISG-NH_2	$C_{26}H_{50}N_8O_8$	602.77	603.3824	603.3814	1.6573	38.3	95
LM13a	*Cyc*(LSKISGGIGPLVIPv)	$C_{68}H_{118}N_{16}O_{17}$	1431.79	1431.8934	1431.8863	4.9585	6.1	95
LM13b	*Cyc*(LSKISGGIGPLVIPV)	$C_{68}H_{118}N_{16}O_{17}$	1431.79	1431.8934	1431.8873	4.2601	1.0	95

Marfey's Analysis of cyclic peptides

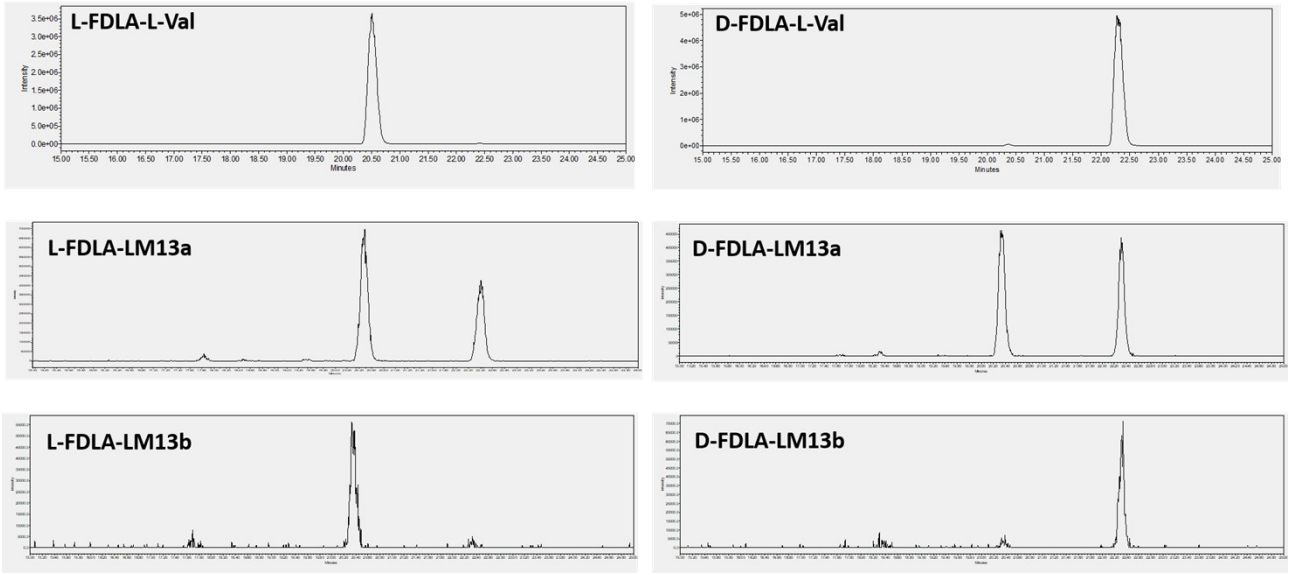


Figure S2. Extracted ion chromatogram of Marfey's derivatives (L-/D-FDLA) of L-Val, LM13a and LM13b at 368 Da in negative ion mode.

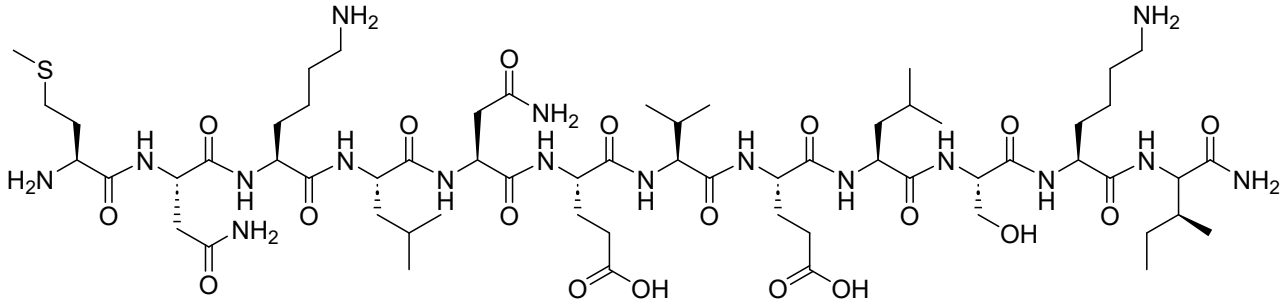
Table S2: Marfey's analysis of Valine amino acid in LM13a and LM13b

	L-FDLA derivative t_R (min)	D-FDLA derivative t_R (min)
L-Val	20.5	22.5
LM13a	20.5	20.5
	22.5	22.5
LM13b	20.5	22.5

LM13 contains two valine residues. The Marfey's analysis show that the major compound LM13a has both l- and d-Valine residues within its structure, whereas the minor compound LM13b has only l-Valine within its structure. The d-Valine in LM13a is the result of the epimierization of the valine residue at the point of macrocyclization.

Structures, LC chromatograms, and HRMS spectra of the synthesized peptides

A) **LM1**



Chemical Formula: $C_{61}H_{109}N_{17}O_{19}S$
Exact Mass: 1415.7806

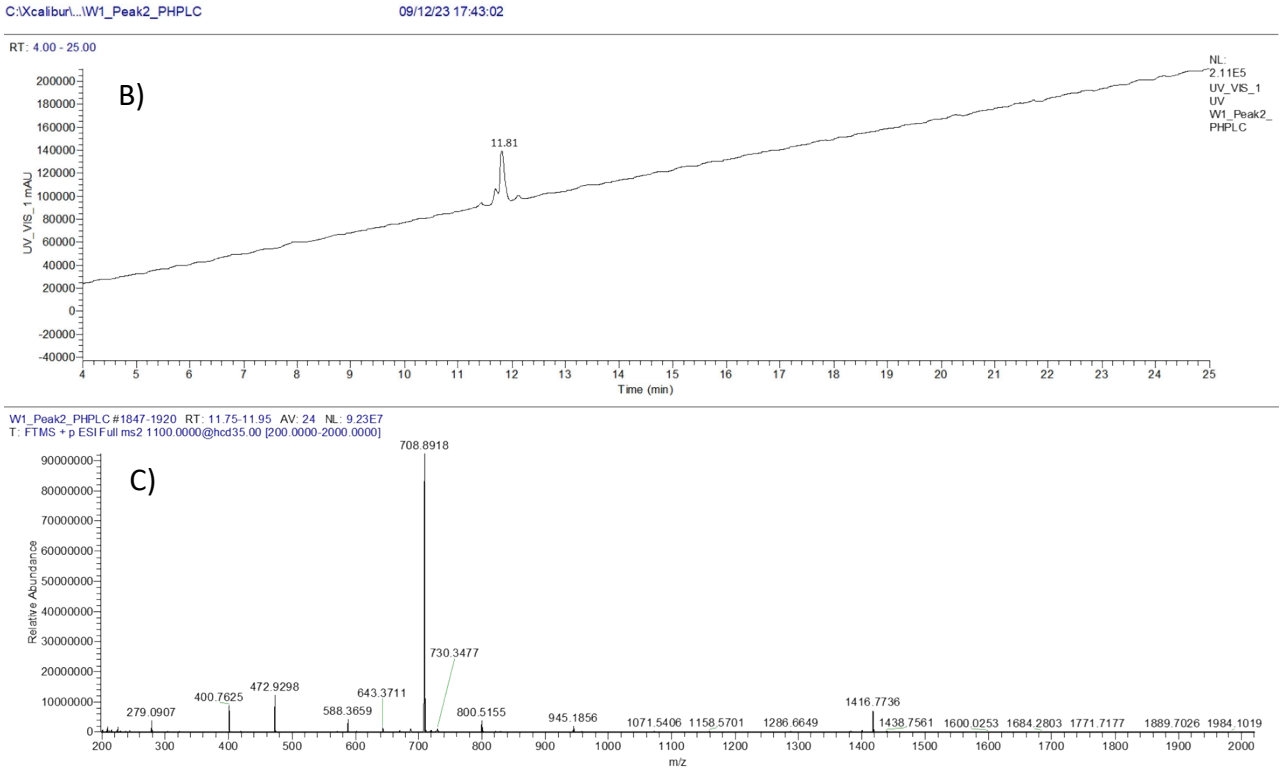
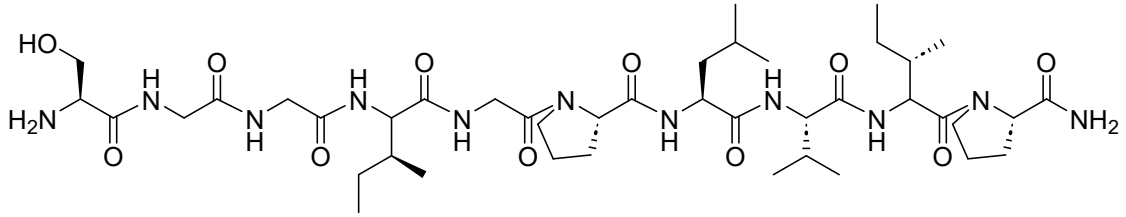


Figure S3: A) LM1 peptide chemical structure, **B)** LC-UV chromatogram of LM1 at 220nm; t_R = 11.81 min; 76% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM1 peak

Table S3: MS peaks and MS^2 fragments observed for LM1

Ion	Found	Expected	Δm
MNKLNEVELSKI-NH_2 + H^+	1416.7736	1416.7879	10.1 ppm
MNKLNEVELSKI-NH_2 + Na^+	1438.7561	1438.7699	9.6 ppm
MNKLNEVELSKI-NH_2 + $2H^+$	708.8918	708.8976	8.2 ppm
LM1 I-NH_2	1286.6649	1286.6773	9.6 ppm
LM1 KI-NH_2	1158.5701	1158.5824	10.6 ppm
LM1 SKI-NH_2	1071.5406	1071.5503	9.1 ppm

A) **LM2**



Chemical Formula: $C_{42}H_{73}N_{11}O_{11}$
Exact Mass: 907.5491

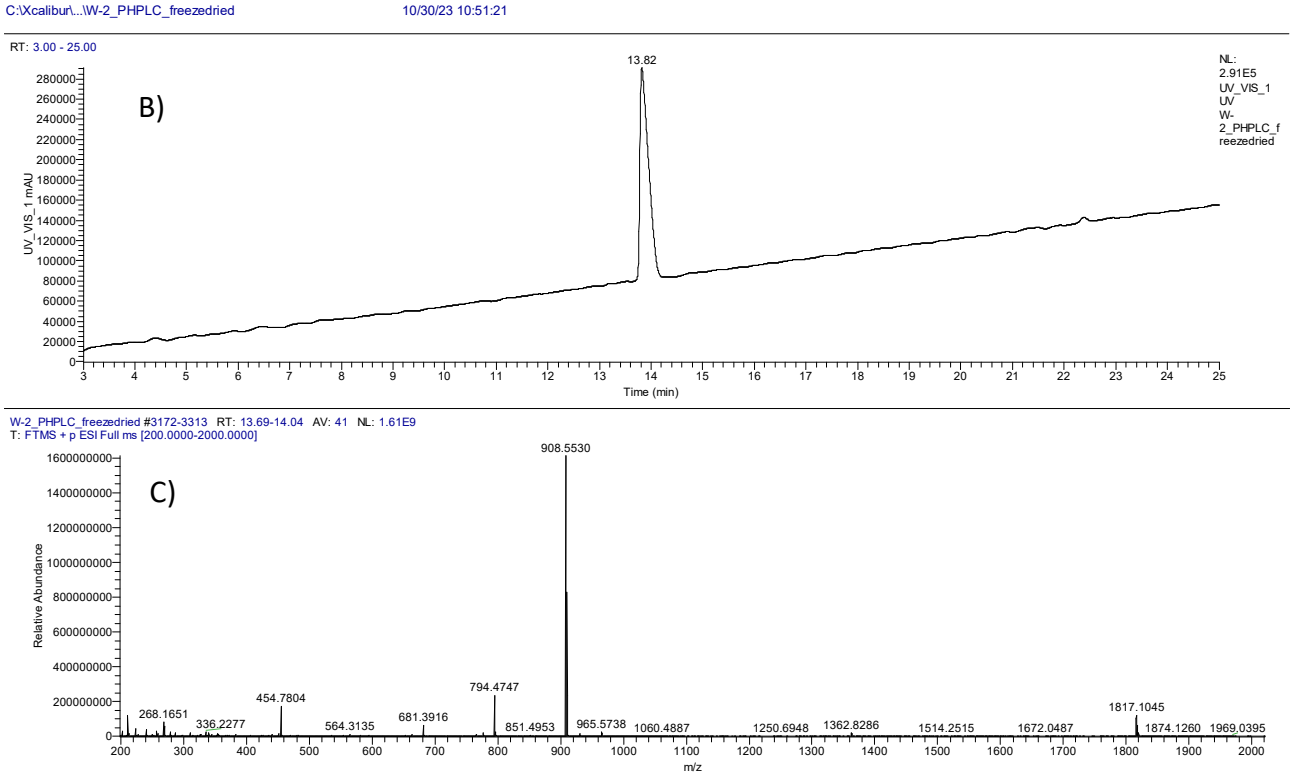
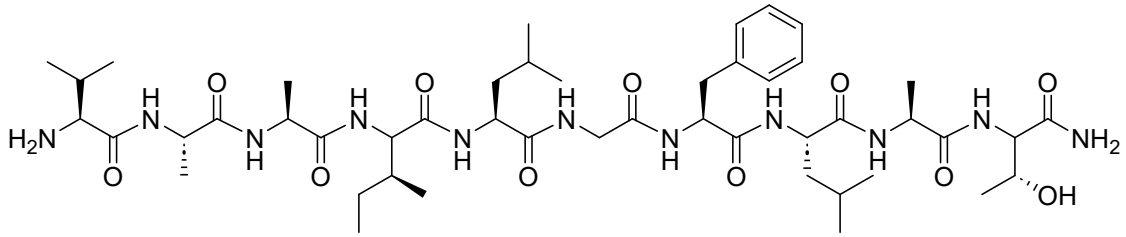


Figure S4: A) LM2 peptide chemical structure, **B)** LC-UV chromatogram of LM2 at 220nm; t_R = 13.82 min; 99% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM2 peak.

Table S4: MS peaks and MS^2 fragments observed for LM2

Ion	**Found**	**Expected**	**Δm**
SGGIGPLVIP-NH_2 + H^+	908.5530	908.5564	3.7 ppm
$(SGGIGPLVIP\text{-}NH_2)_2$ + H^+	1816.1020	1816.1055	1.9 ppm
SGGIGPLVIP-NH_2 + $2H^+$	454.7804	454.7819	3.3 ppm
LM2 P-NH_2	794.4747	794.4771	3.0 ppm
LM2 IP-NH_2	681.3916	681.3931	2.2 ppm
LM2 VIP-NH_2 H_2O	564.3135	564.3141	1.1 ppm

A) **LM3**



Chemical Formula: $C_{47}H_{79}N_{11}O_{11}$
Exact Mass: 973.5961

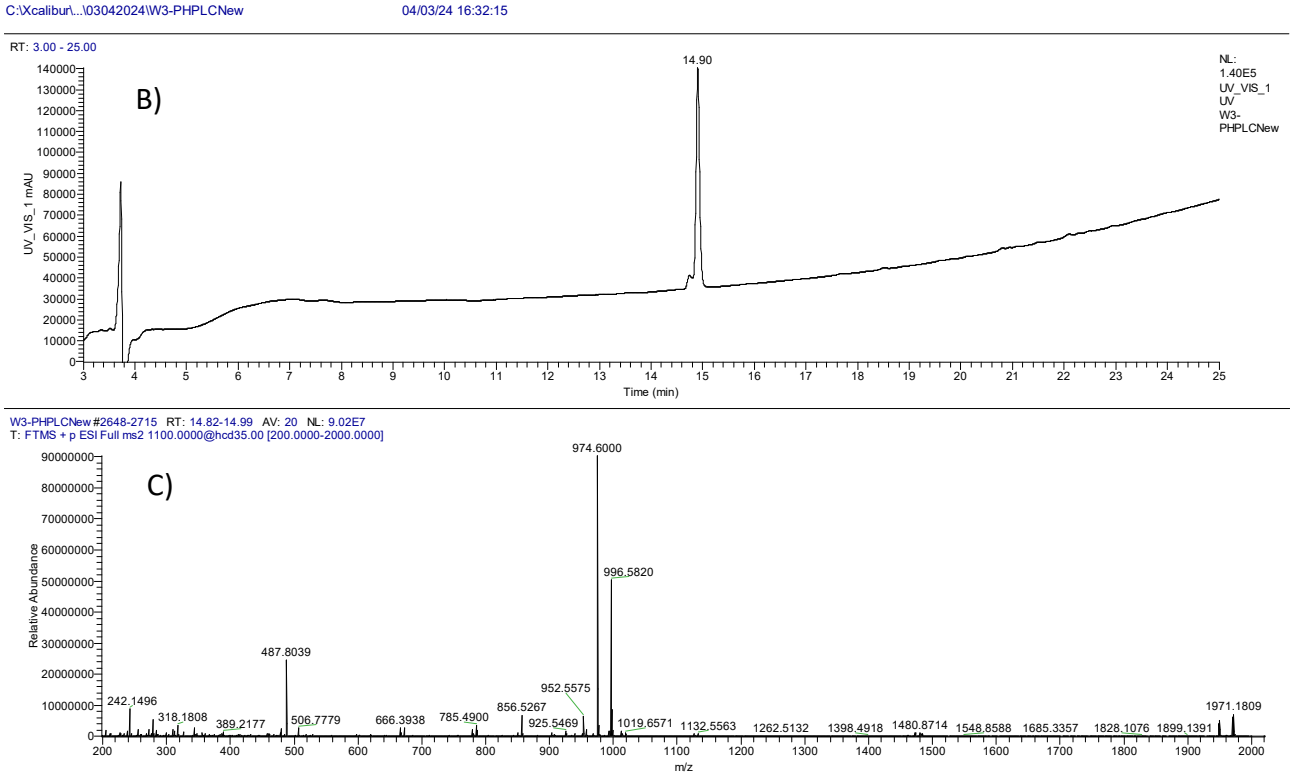
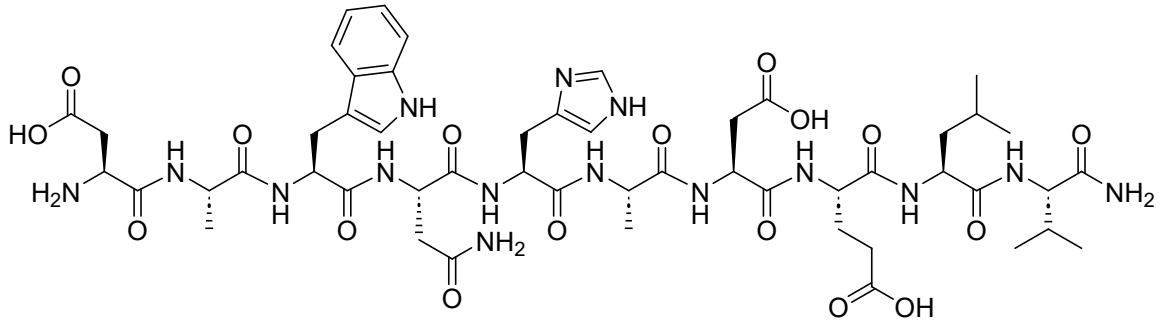


Figure S5: A) LM3 peptide chemical structure, **B)** LC-UV chromatogram of LM3 at 220nm; t_R = 14.90 min; 96% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM3 peak.

Table S5: MS peaks and MS^2 fragments observed for LM3

Ion	**Found**	**Expected**	**Δm**
VAAILGFLAT-NH_2 + H^+	974.6000	974.6033	3.4 ppm
VAAILGFLAT-NH_2 + Na^+	996.5820	996.5853	3.3 ppm
$(VAAILGFLAT\text{-}NH_2)_2$ + H^+	1949.1989	1949.2028	2.0 ppm
$(VAAILGFLAT\text{-}NH_2)_2$ + Na^+	1971.1816	1971.1847	1.6 ppm
VAAILGFLAT-NH_2 + $2H^+$	487.8039	487.8053	2.9 ppm
LM3 T-NH_2	856.5267	856.5291	2.8 ppm
LM3 AT-NH_2	785.4900	785.4920	2.5 ppm
LM3 LAT-NH_2	672.4063	672.4080	2.5 ppm

A) **LM4**



Chemical Formula: $C_{51}H_{73}N_{15}O_{17}$
Exact Mass: 1167.5309

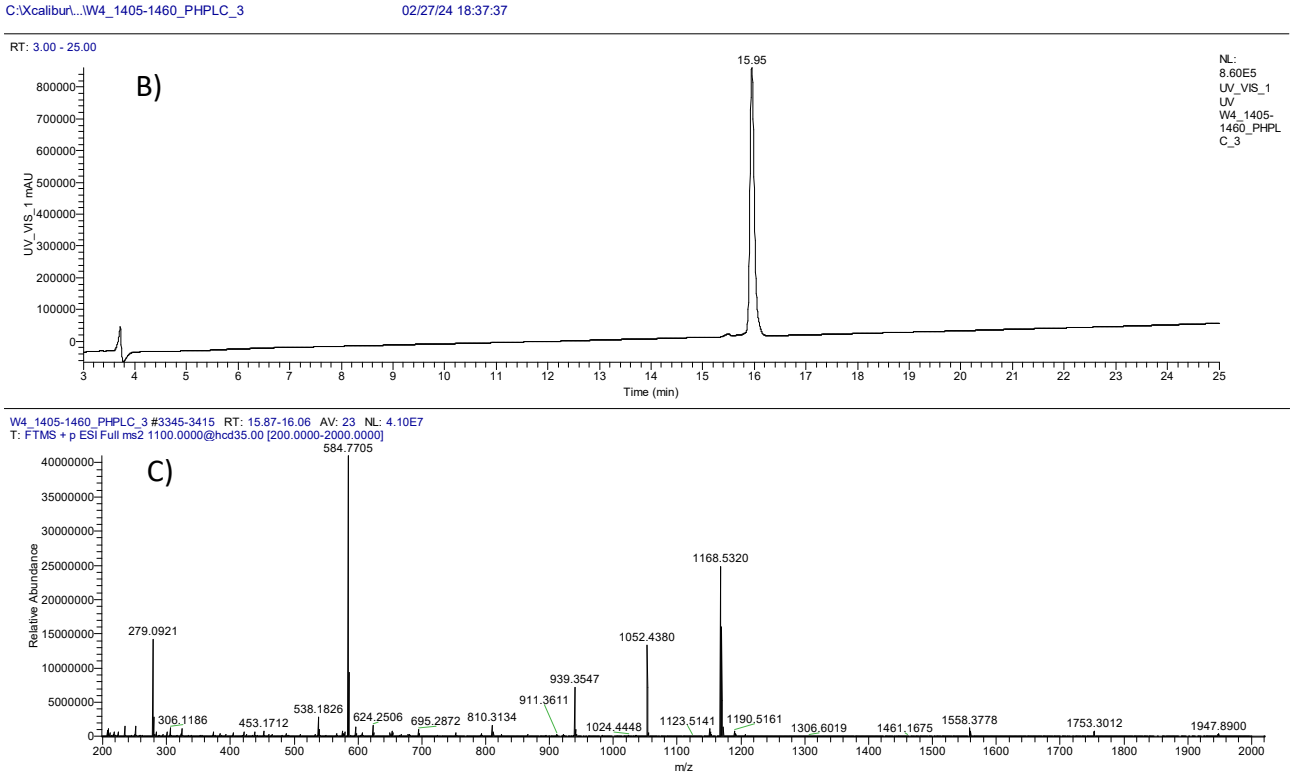
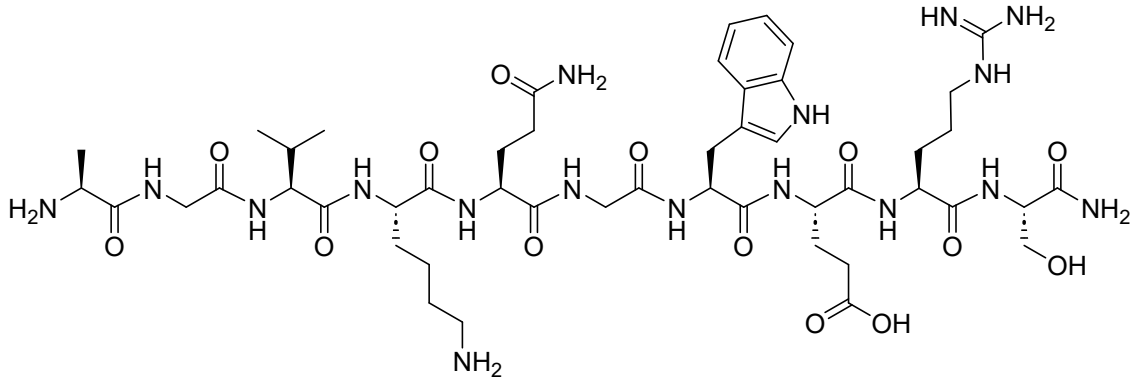


Figure S6: A) LM4 peptide chemical structure, **B)** LC-UV chromatogram of LM4 at 220nm; t_R = 15.95 min; 97% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM4 peak.

Table S6: MS peaks and MS^2 fragments observed for LM4

Ion	**Found**	**Expected**	**Δm**
DAWNHADELV-NH_2 + H^+	1168.5320	1168.5382	5.3 ppm
DAWNHADELV-NH_2 + Na^+	1190.5161	1190.5202	3.4 ppm
DAWNHADELV-NH_2 + $2H^+$	584.7705	584.7727	3.8 ppm
LM4 V-NH_2	1052.4380	1052.4432	4.9 ppm
LM4 LV-NH_2	939.3547	939.3592	4.8 ppm
LM4 ELV-NH_2	810.3134	810.3166	3.9 ppm
LM4 DELV-NH_2	695.2872	695.2896	3.5 ppm
LM4 ADELV-NH_2	624.2506	624.2525	3.0 ppm

A) **LM5**



Chemical Formula: $C_{48}H_{77}N_{17}O_{14}$
Exact Mass: 1115.5836

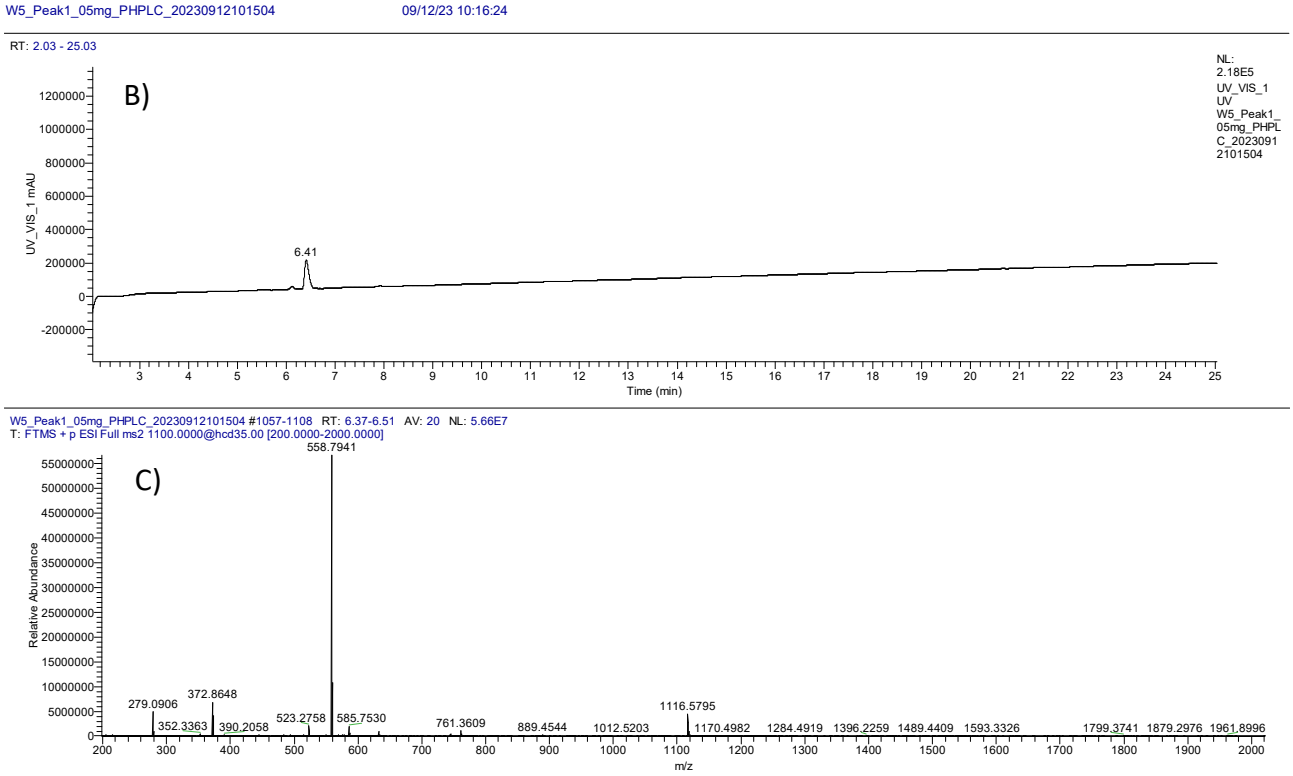
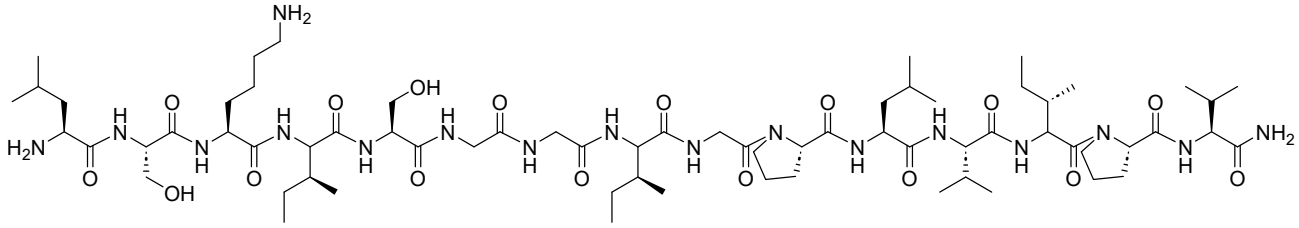


Figure S7: A) LM5 peptide chemical structure, **B)** LC-UV chromatogram of LM5 at 220nm; t_R = 6.41 min; 99% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM5 peak.

Table S7: MS peaks and MS^2 fragments observed for LM5

Ion	**Found**	**Expected**	**Δm**
AGVKQGWERS-NH_2 + H^+	1116.5795	1116.5909	10.2 ppm
AGVKQGWERS-NH_2 + $2H^+$	558.7941	558.7991	8.9 ppm
LM5 S-NH_2	1012.5203	1012.5323	11.9 ppm
LM5 AGV + H^+	889.4544	889.4639	10.7 ppm
LM5 AGVK + H^+	761.3609	761.3690	10.6 ppm
LM5 AGVKQGW + H^+	390.2058	390.2096	9.7 ppm

A) **LM6**



Chemical Formula: $C_{68}H_{120}N_{16}O_{18}$
Exact Mass: 1448.8967

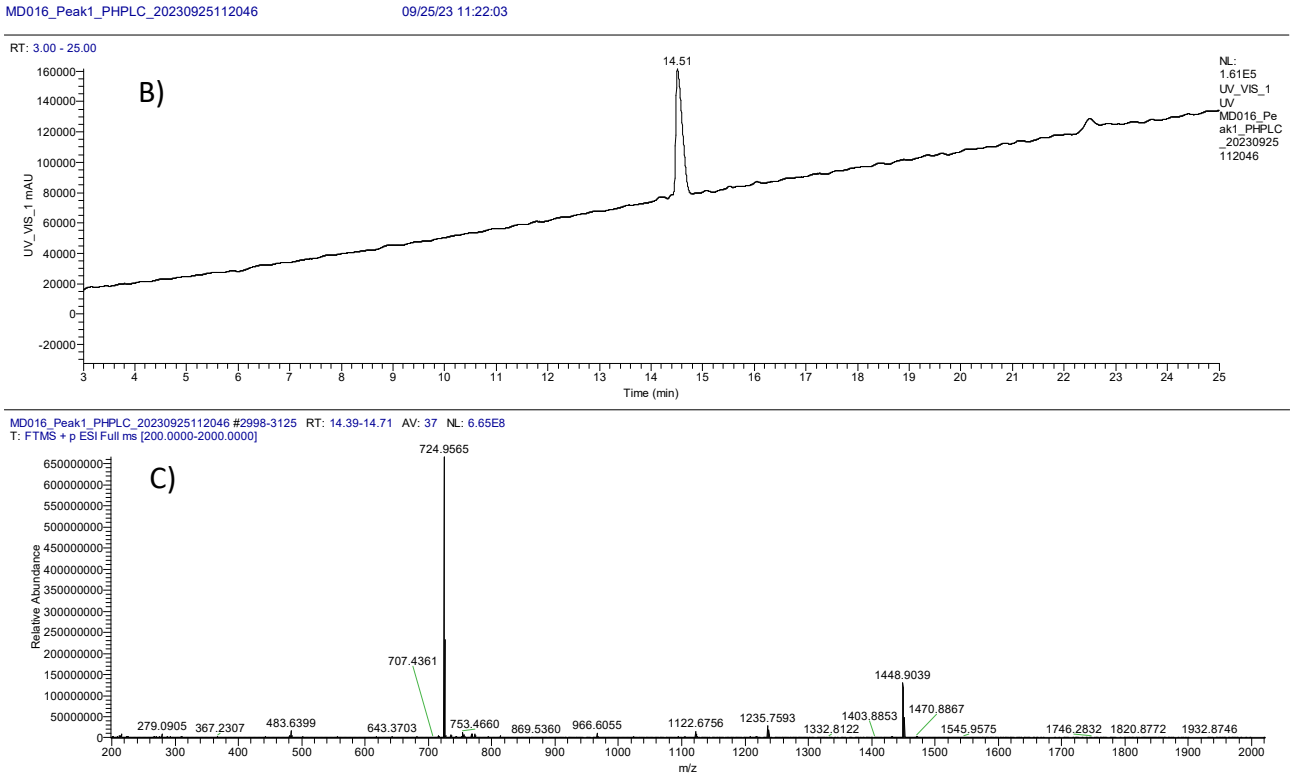
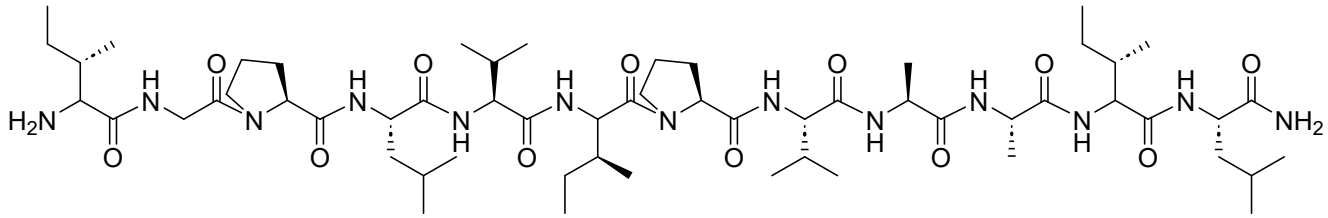


Figure S8: A) LM6 peptide chemical structure, **B)** LC-UV chromatogram of LM6 at 220nm; t_R = 14.51 min; 98% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM6 peak.

Table S8: MS peaks and MS^2 fragments observed for LM6

Ion	**Found**	**Expected**	**Δm**
LSKISGGIGPLVIPV-NH_2 + H^+	1448.9039	1448.9199	11.0 ppm
LSKISGGIGPLVIPV-NH_2 + Na^+	1470.8867	1470.9019	10.3 ppm
LSKISGGIGPLVIPV-NH_2 + $2H^+$	724.9565	724.9636	9.8 ppm
LM6 CO-NH_2	1403.8853	1403.8985	9.4 ppm
LM6 V-NH_2	1332.8122	1332.8250	9.6 ppm
LM6 PV-NH_2	1235.7593	1235.7722	10.4 ppm
LM6 IPV-NH_2	1122.6756	1122.6882	11.2 ppm
LM6 IGPLVIPV-NH_2	643.3703	643.3774	11.0 ppm

A) **LM7**



Chemical Formula: $C_{58}H_{103}N_{13}O_{12}$
Exact Mass: 1173.7849

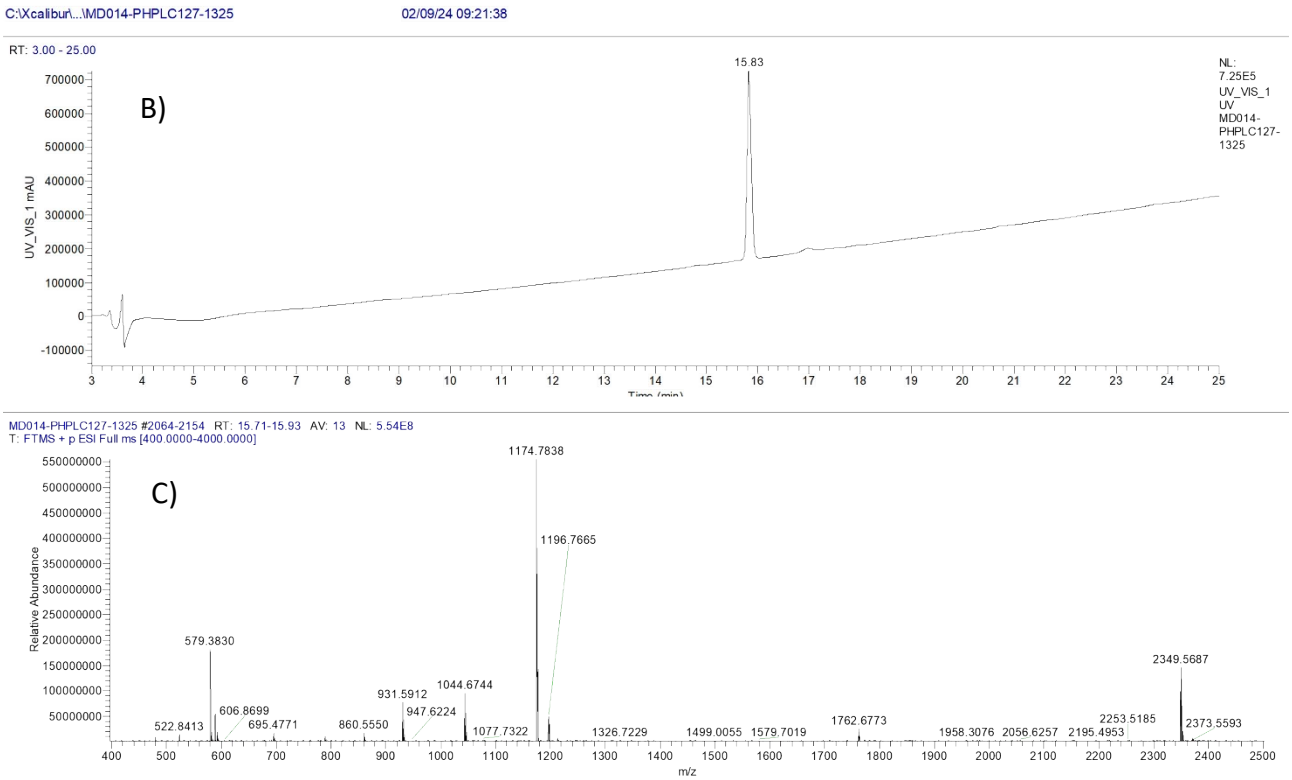
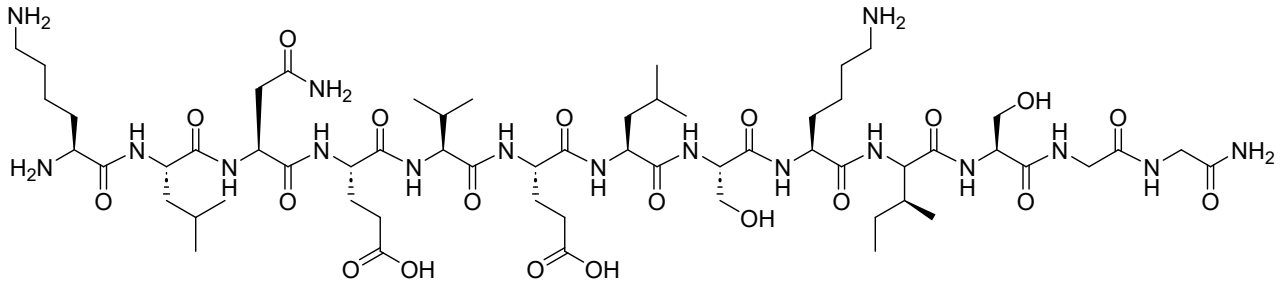


Figure S9: A) LM7 peptide chemical structure, **B)** LC-UV chromatogram of LM7 at 220nm; t_R = 15.83 min; 97% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM7 peak.

Table S9: MS peaks and MS^2 fragments observed for LM7

Ion	**Found**	**Expected**	**Δm**
IGPLVIPVAAIL-NH_2 + H^+	1174.7838	1174.7922	7.2 ppm
IGPLVIPVAAIL-NH_2 + Na^+	1196.7665	1196.7742	6.4 ppm
IGPLVIPVAAIL-NH_2 + K^+	1212.7397	1212.7481	6.9 ppm
$(IGPLVIPVAAIL\text{-}NH_2)_3$ + $2H^+$	1762.1749	1762.1864	6.5 ppm
$(IGPLVIPVAAIL\text{-}NH_2)_2$ + H^+	2349.5687	2349.5805	5.0 ppm
IGPLVIPVAAIL-NH_2 + $2H^+$	587.8960	587.8998	6.5 ppm
LM7 L-NH_2	1044.6744	1044.6816	6.9 ppm
LM7 IL-NH_2	931.5912	931.5976	6.9 ppm
LM7 AIL-NH_2	860.5550	860.5605	6.4 ppm
LM7 AAIL-NH_2	789.5181	789.5233	6.6 ppm

A) **LM8**



Chemical Formula: $C_{59}H_{105}N_{17}O_{20}$
Exact Mass: 1371.7722

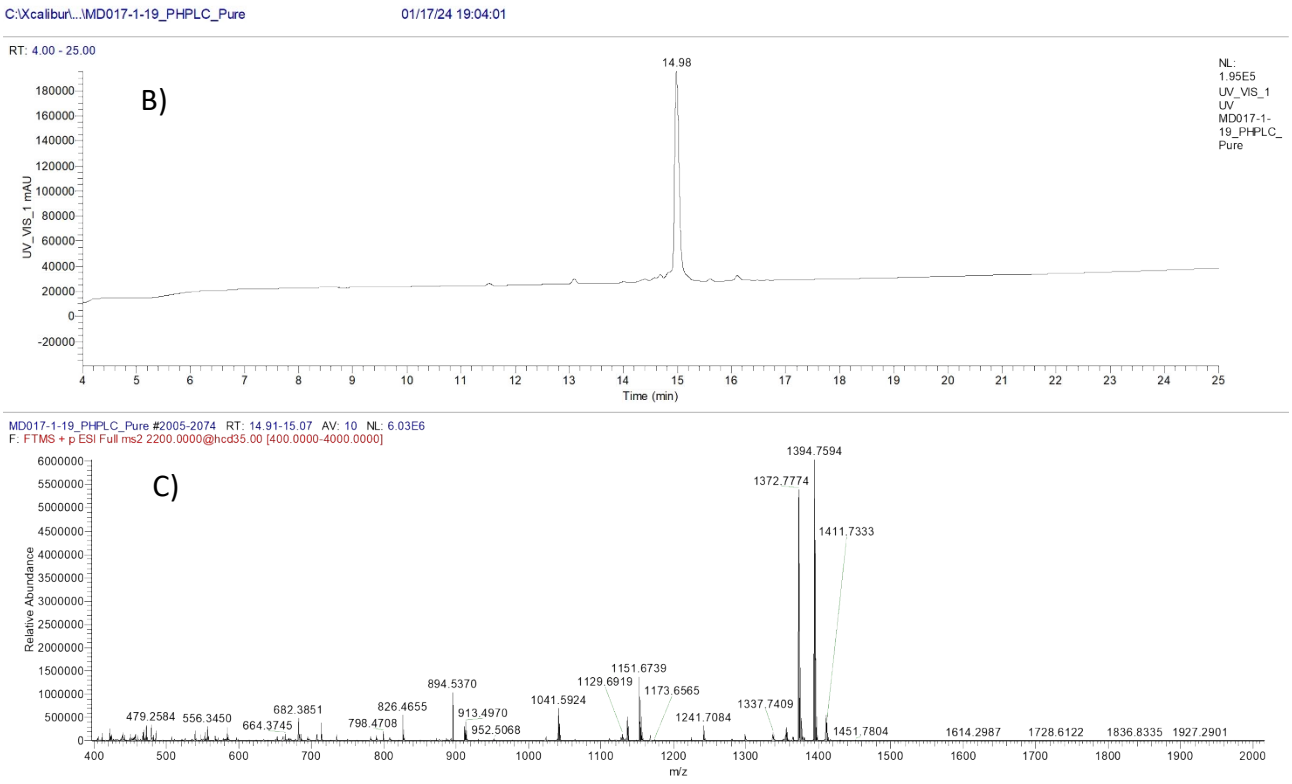
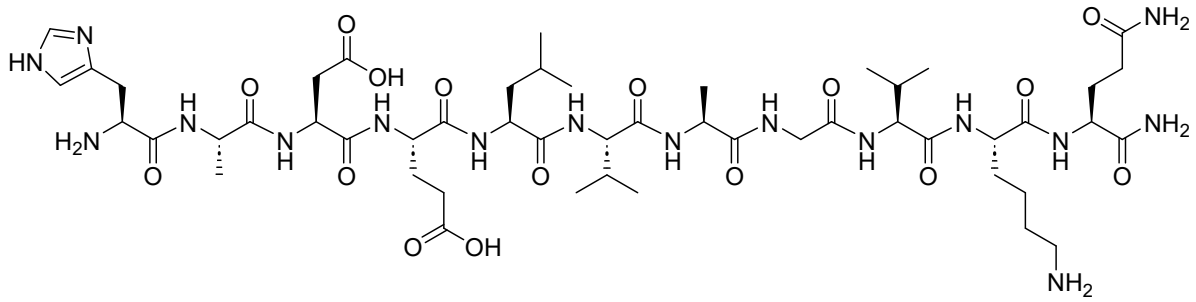


Figure S10: A) LM8 peptide chemical structure, **B)** LC-UV chromatogram of LM8 at 220nm; t_R = 14.98 min; 98% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM8 peak.

Table S10: MS peaks and MS^2 fragments observed for LM8

Ion	**Found**	**Expected**	**Δm**
KLNEVELSKISGG-NH_2 + H^+	1372.7774	1372.7795	1.5 ppm
KLNEVELSKISGG-NH_2 + Na^+	1394.7594	1394.7614	1.4 ppm
KLNEVELSKISGG-NH_2 + K^+	1410.7302	1410.7354	3.7 ppm
LM8 GG-NH_2	1241.7084	1241.7100	1.3 ppm
LM8 ISGG-NH_2	1041.5924	1041.5939	1.4 ppm
LM8 KISGG-NH_2	913.4970	913.4990	2.2 ppm
LM8 SKISGG-NH_2	826.4655	826.4669	1.7 ppm

A) **LM9**



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Exact Mass: 1164.6251

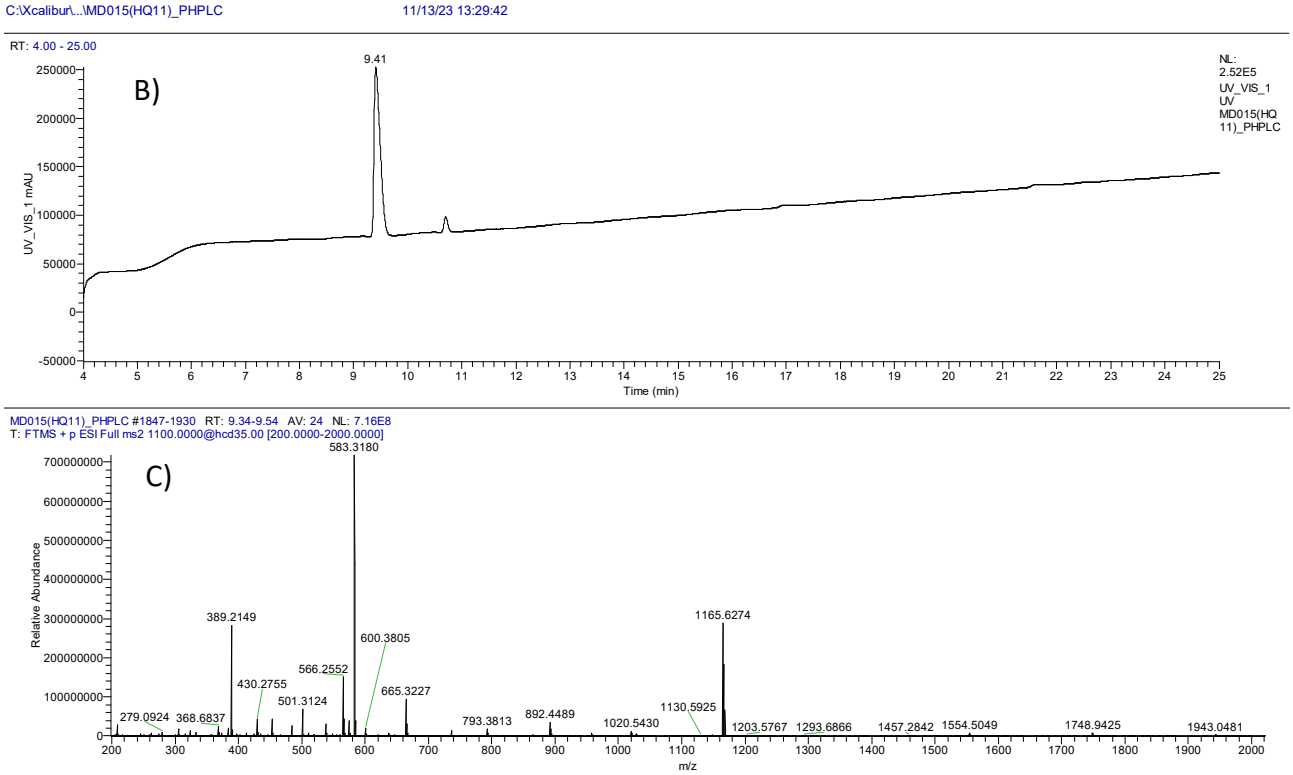
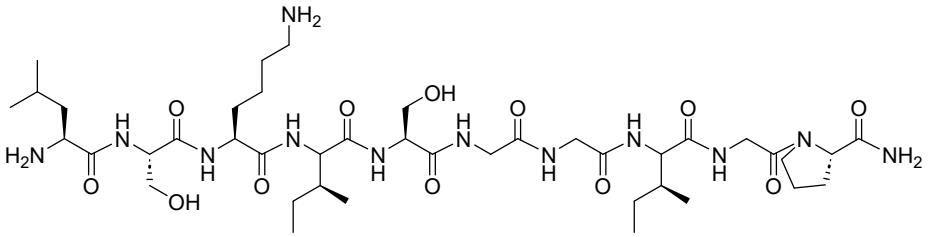


Figure S11: A) LM9 peptide chemical structure, **B)** LC-UV chromatogram of LM9 at 220nm; t_R = 9.41 min; 95% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM9 peak.

Table S11: MS peaks and MS^2 fragments observed for LM9

Ion	Found	Expected	Δm
HADELVAGVKQ-NH_2 + H^+	1165.6274	1165.6324	4.3 ppm
HADELVAGVKQ-NH_2 + $2H^+$	583.3180	583.3199	3.3 ppm
LM9 Q-NH_2	1020.5430	1020.5473	4.2 ppm
LM9 KQ-NH_2	892.4489	892.4524	3.9 ppm
LM9 VKQ-NH_2	793.3813	793.3839	3.3 ppm
LM9 GVKQ-NH_2	736.3600	736.3625	3.4 ppm
LM9 AGVKQ-NH_2	665.3227	665.3254	4.1 ppm
LM9 VAGVKQ-NH_2	566.2552	566.2570	3.2 ppm
LM9 LVAGVKQ-NH_2	453.1715	453.1729	3.1 ppm
LM9 HADEL + H^+	600.3805	600.3828	3.8 ppm
LM9 HADELV + H^+	501.3124	501.3144	4.0 ppm
LM9 HADELVA + H^+	430.2755	430.2773	4.2 ppm

A) **LM10**



Chemical Formula: $C_{41}H_{74}N_{12}O_{12}$
Exact Mass: 926.5549

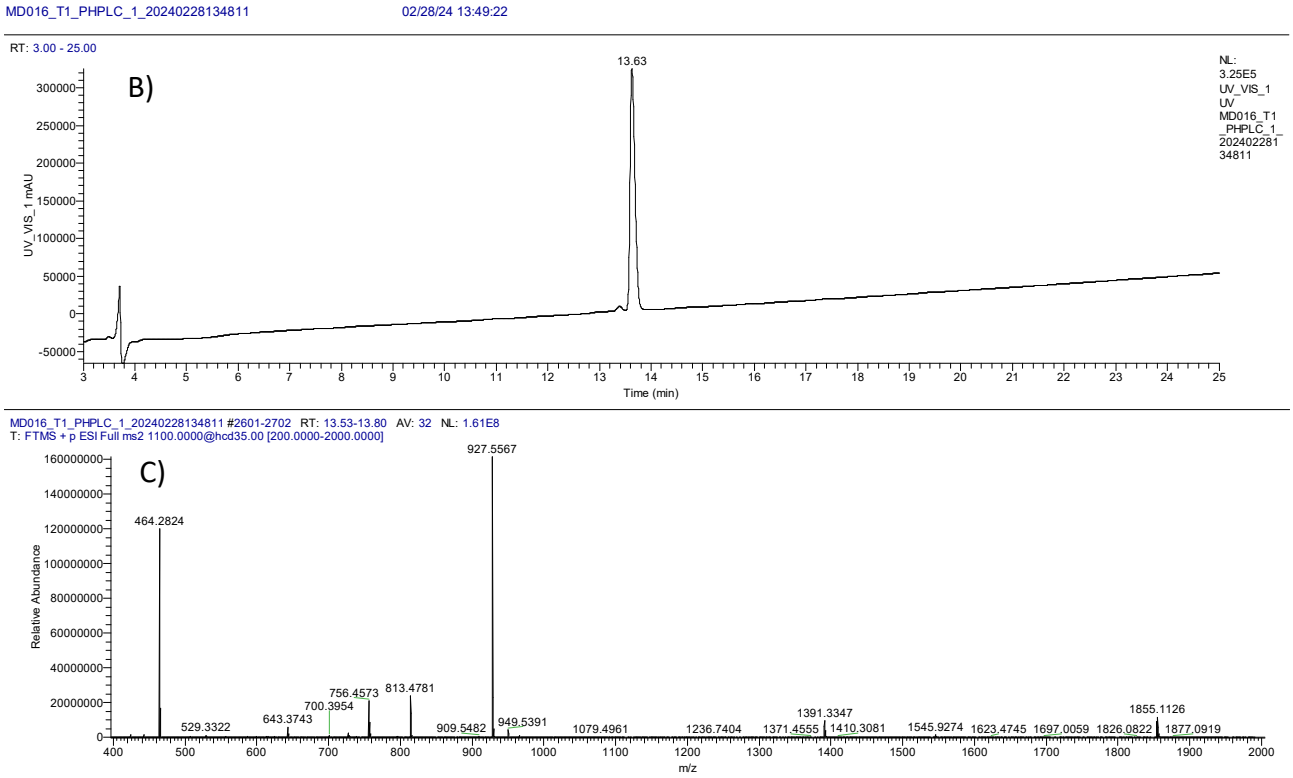
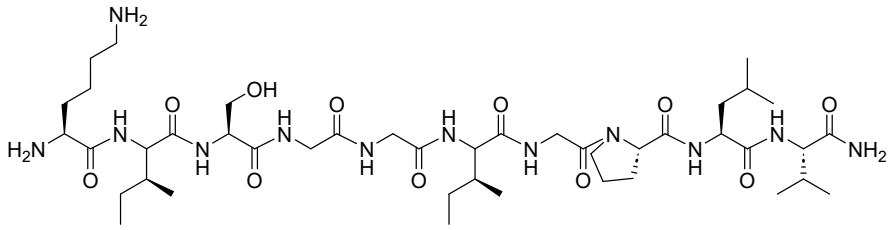


Figure S12: A) LM10 peptide chemical structure, **B)** LC-UV chromatogram of LM10 at 220nm; t_R = 13.63 min; 96% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM10 peak.

Table S12: MS peaks and MS^2 fragments observed for LM10

Ion	Found	Expected	Δm
LSKISGGIGP-NH_2 + H^+	927.5567	927.5622	5.9 ppm
LSKISGGIGP-NH_2 + Na^+	949.5391	949.5442	5.4 ppm
(LSKISGGIGP-NH_2)$_3$ + $2H^+$	1391.3347	1391.3414	4.8 ppm
(LSKISGGIGP-NH_2)$_2$ + H^+	1854.1102	1854.1172	3.8 ppm
LSKISGGIGP-NH_2 + $2H^+$	464.2824	464.2848	5.2 ppm
LM10 P-NH_2	813.4781	813.4829	5.9 ppm
LM10 GP-NH_2	756.4573	756.4615	5.6 ppm
LM10 IGP-NH_2	643.3743	643.3774	4.8 ppm
LM10 GGIGP-NH_2	529.3322	529.3345	4.3 ppm

A) **LM11**



Chemical Formula: $C_{43}H_{78}N_{12}O_{11}$
Exact Mass: 938.5913

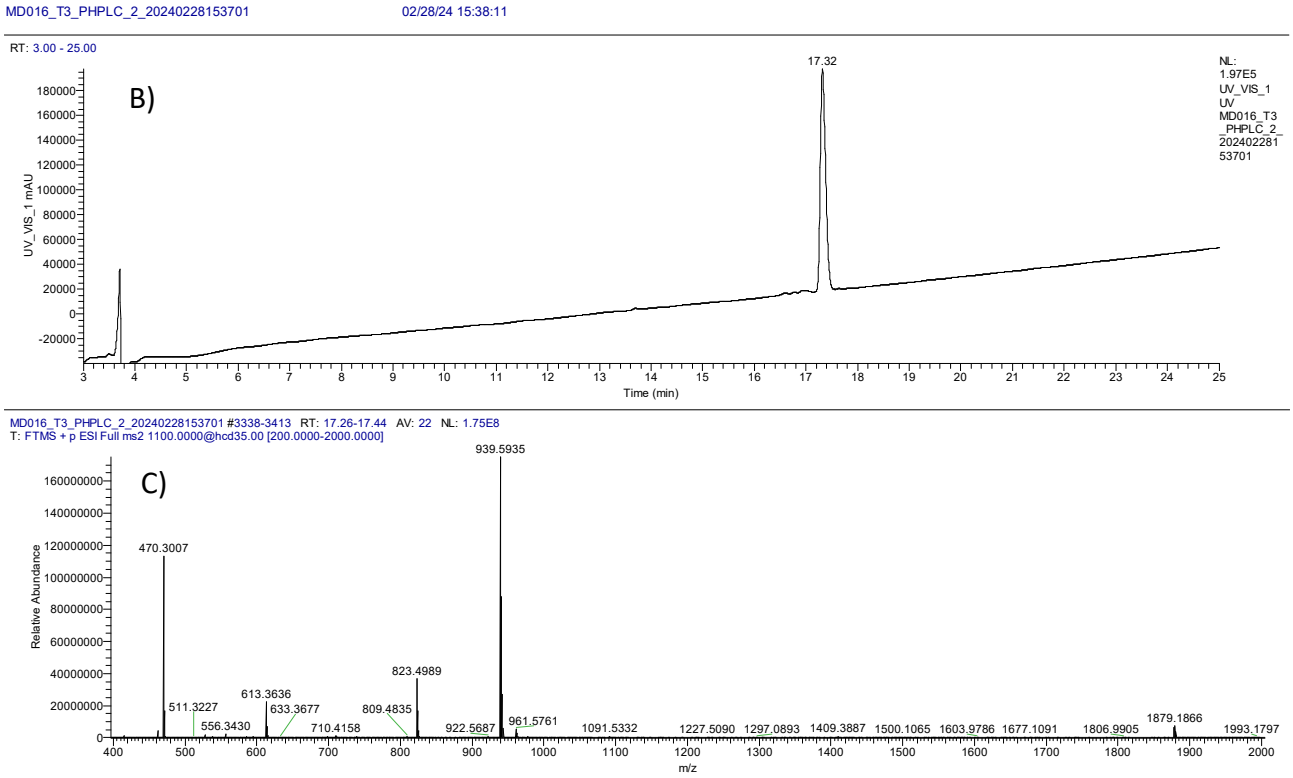
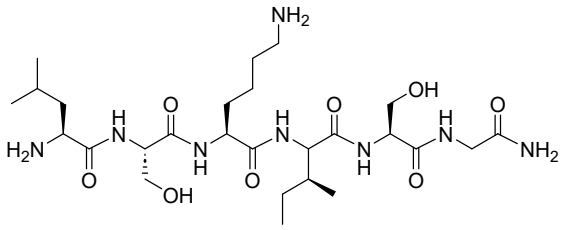


Figure S13: A) LM11 peptide chemical structure, **B)** LC-UV chromatogram of LM11 at 220nm; t_R = 17.32 min; 97% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM11 peak.

Table S13: MS peaks and MS^2 fragments observed for LM11

Ion	**Found**	**Expected**	**Δm**
KISGGIGPLV-NH_2 + H^+	939.5935	939.5986	5.4 ppm
KISGGIGPLV-NH_2 + Na^+	961.5761	961.5806	4.7 ppm
$(KISGGIGPLV\text{-}NH_2)_2$ + H^+	1878.1840	1878.1899	3.1 ppm
KISGGIGPLV-NH_2 + $2H^+$	470.3007	470.3030	4.9 ppm
LM11 V-NH_2	823.5037	823.4989	5.8 ppm
LM11 LV-NH_2	710.4158	710.4196	5.3 ppm
LM11 PLV-NH_2	613.3636	613.3668	5.2 ppm
LM11 GPLV-NH_2	556.3430	556.3454	4.3 ppm

A) **LM12**



Chemical Formula: $C_{26}H_{50}N_8O_8$
Exact Mass: 602.3752

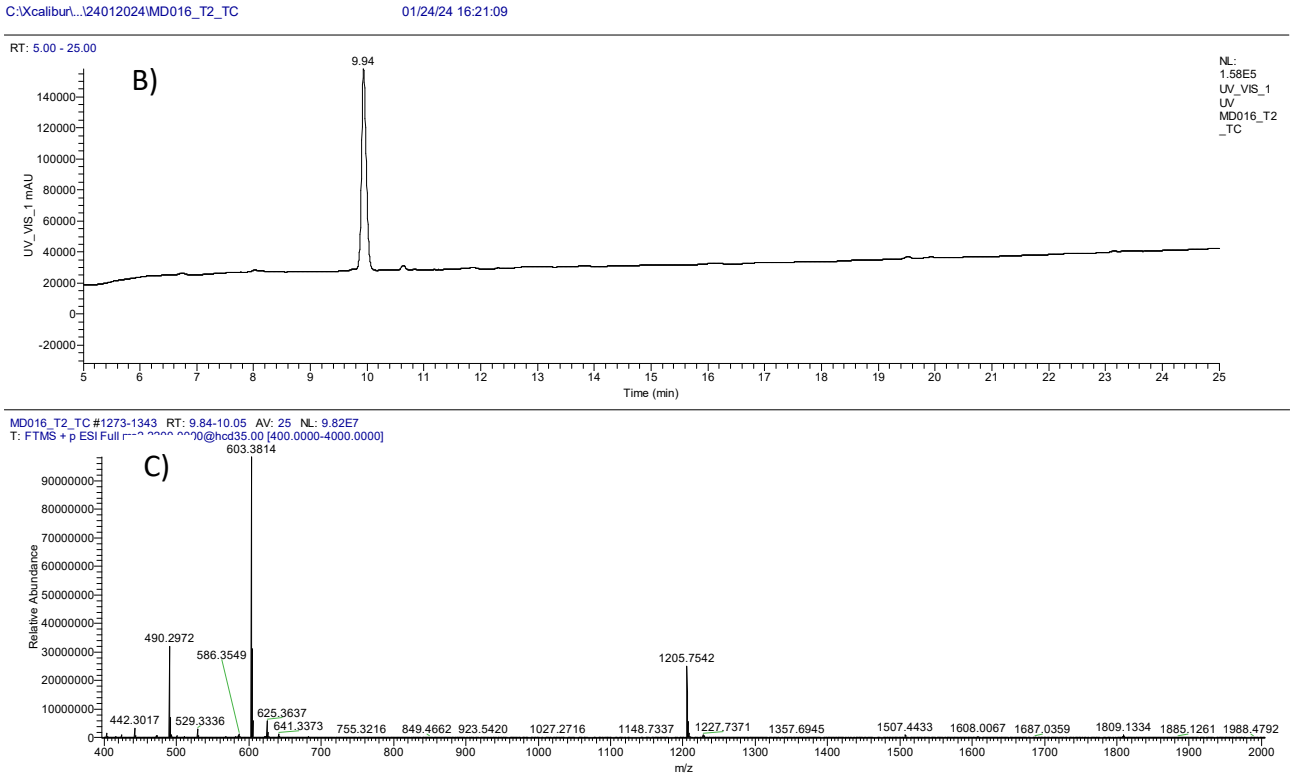
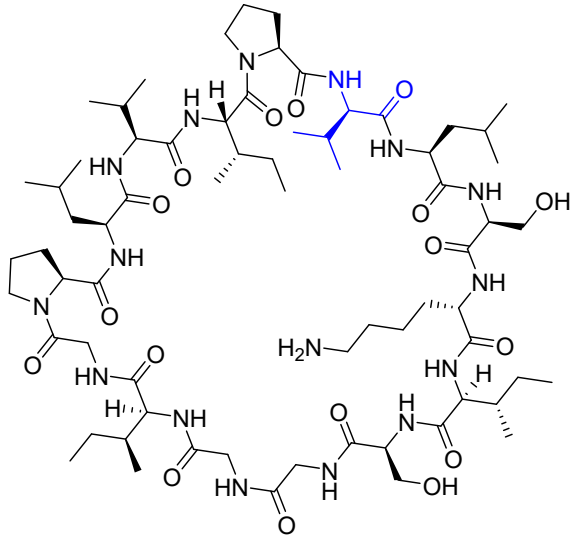


Figure S14: A) LM12 peptide chemical structure, **B)** LC-UV chromatogram of LM12 at 220nm; t_R = 9.94 min; 95% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM12 peak.

Table S14: MS peaks and MS^2 fragments observed for LM12

Ion	**Found**	**Expected**	**Δm**
LSKISG-NH_2 + H^+	603.3814	603.3824	1.7 ppm
LSKISG-NH_2 + Na^+	625.3637	625.3644	1.1 ppm
LSKISG-NH_2 + K^+	641.3373	641.3384	1.7 ppm
(LSKISG-NH_2)$_2$ + H^+	1205.7542	1205.7576	2.8 ppm
LM12 NH_2	586.3549	586.3559	1.7 ppm
LM12 G-NH_2	529.3336	529.3345	1.7 ppm
LM12 SG-NH_2	442.3017	442.3024	1.6 ppm
LM12 L + H^+	490.2972	490.2984	2.4 ppm

A) **LM13a**



Chemical Formula: $C_{68}H_{118}N_{16}O_{17}$
Exact Mass: 1430.88609

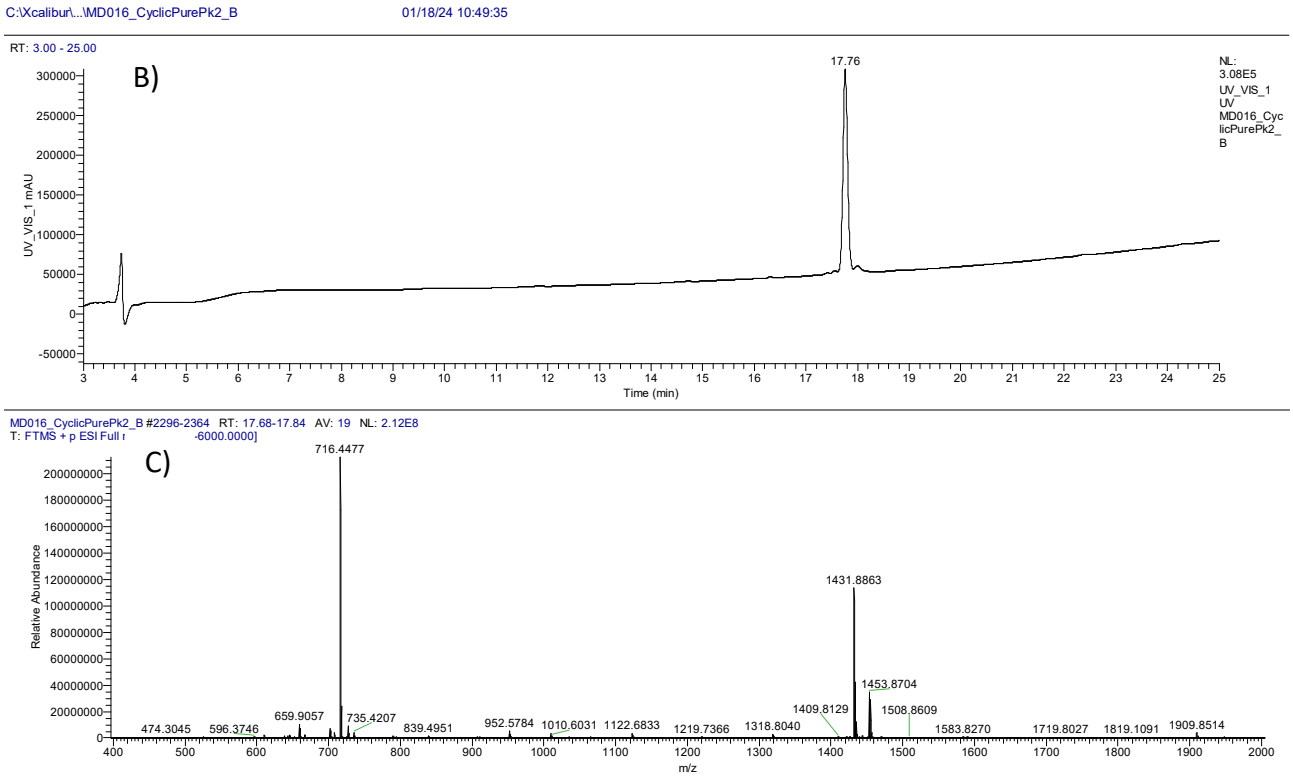
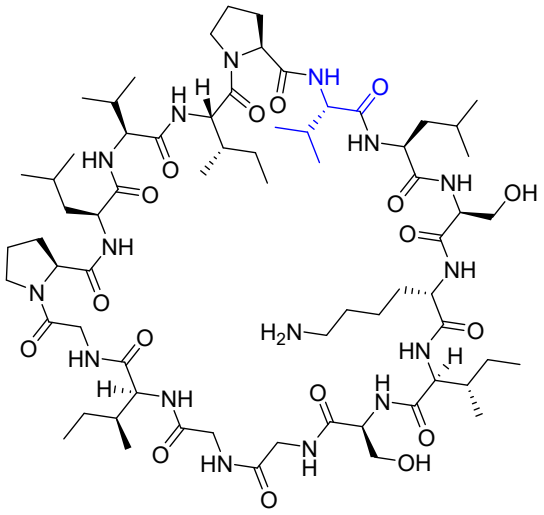


Figure S15: A) LM13a peptide chemical structure, **B)** LC-UV chromatogram of LM13a at 220nm; t_R = 17.76 min; 95% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM13a peak.

Table S15: MS peaks observed for LM13a

Ion	Found	Expected	Δm
Cyc(LSKISGGIGPLVIPv) + H^+	1431.8863	1431.8934	5.0 ppm
Cyc(LSKISGGIGPLVIPv) + Na^+	1453.8704	1453.8753	3.4 ppm
Cyc(LSKISGGIGPLVIPv) + $2H^+$	716.4477	716.4503	3.6 ppm

A) **LM13b**



Chemical Formula: $C_{68}H_{118}N_{16}O_{17}$
Exact Mass: 1430.88609

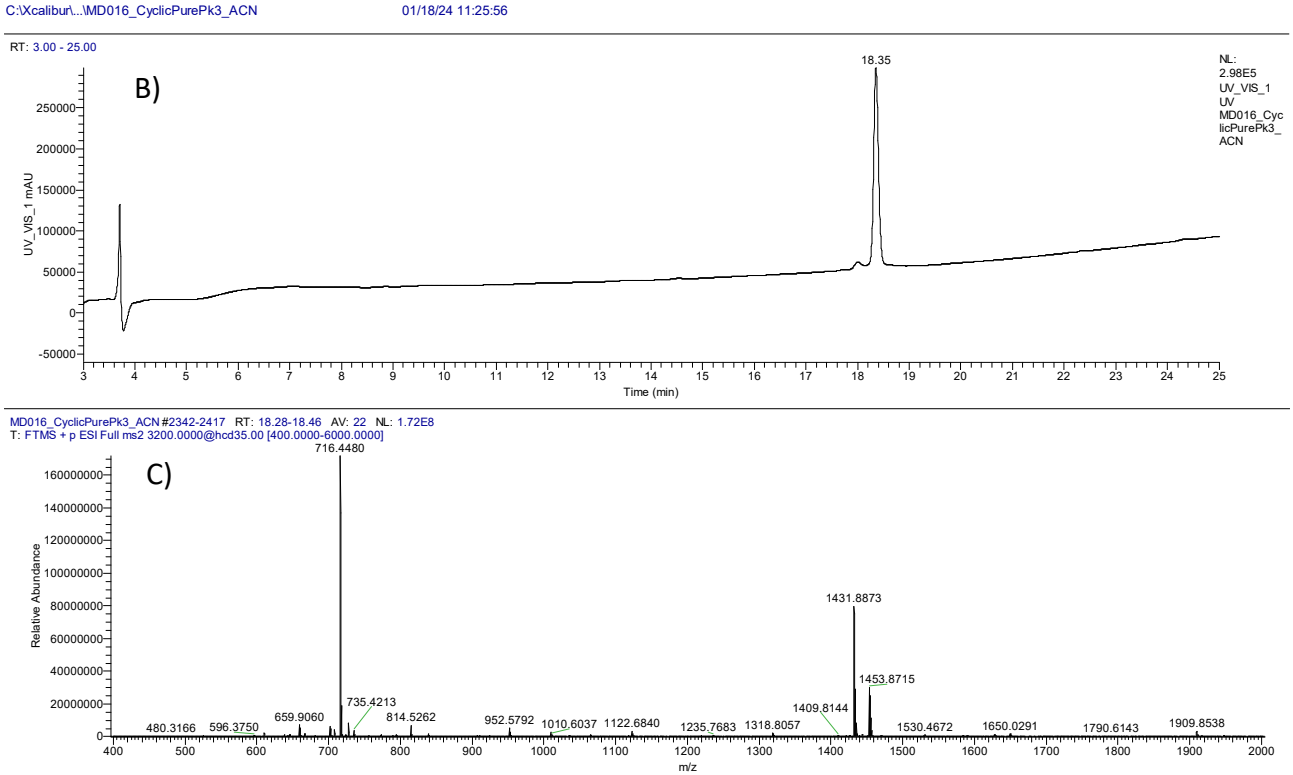


Figure S16: A) LM13b peptide chemical structure, **B)** LC-UV chromatogram of LM13b at 220nm; t_R = 18.35 min; 95% purity, **C)** HRMS-ESI-MS^2 spectrum in the positive mode of LM13b peak.

Table S16: MS peaks observed for LM13a

Ion	**Found**	**Expected**	**Δm**
Cyc(LSKISGGIGPLVIPV) + H^+	1431.8873	1431.8934	4.3 ppm
Cyc(LSKISGGIGPLVIPV) + Na^+	1453.8715	1453.8753	2.6 ppm
Cyc(LSKISGGIGPLVIPV) + $2H^+$	716.4480	716.4503	3.2 ppm

MS/MS fragmentation data of LM6 and its cyclic derivatives LM13a and LM13b

LM6

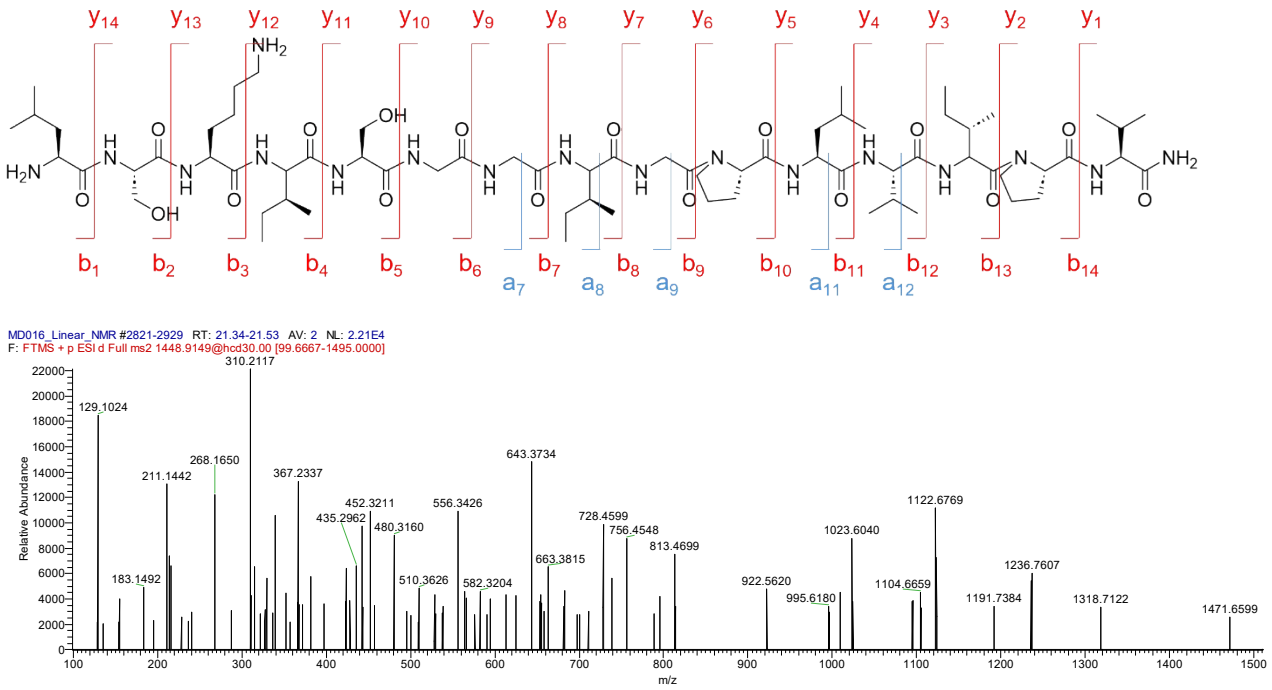


Figure S17: MS^2 fragmentation pattern and MS^2 spectrum of linear peptide LM6.

Table S17: MS^2 fragments observed for LM6 (LSKISGGIGPLVIPV)

Ion	Observed m/z	Ion	Observed m/z
b13	1235.7515	a8	728.4599
b12	1122.6769	b7	643.3734
b11	1023.6040	b5	529.3349
a11	995.6180	b4	442.3050
b9	813.4699	y3	327.2381
a9	785.4830	y2	214.1551
b8	756.4548	y1	117.1025

LM13a

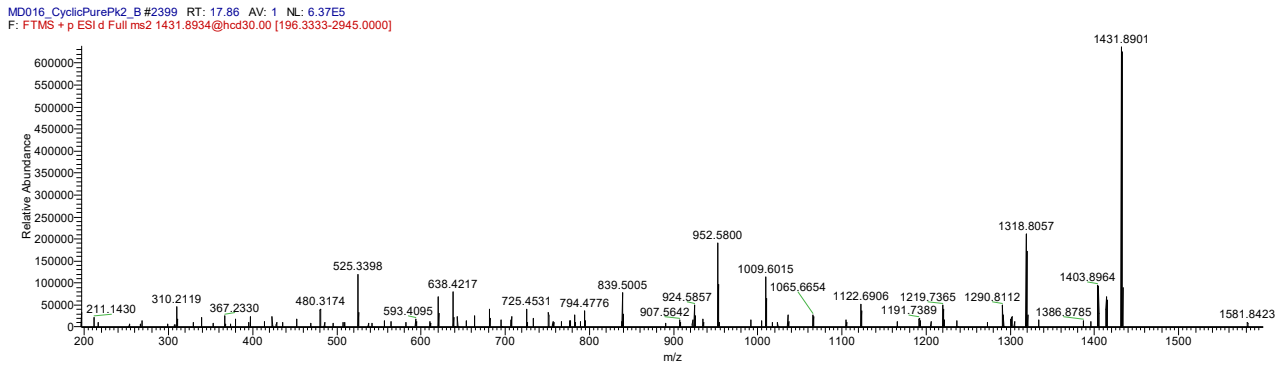


Figure S18: MS^2 fragmentation pattern of cyclic peptide LM13a.

Ion	Additional	Observed m/z	Ion		Observed m/z
LM13a	-CO	1403.8964	LM13a -IVLPGI		839.5005
LM13a -I / -L		1318.8057	LM13a -KSLVPI		794.4776
LM13a -I / -L	-CO	1290.8112	LM13a -IVLPGIGG		725.4554
LM13a -VL / -IV / -LV		1219.7365	LM13a -IVLPGIGGS		638.4217
LM13a -VL -IV / -LV	-CO	1191.7389	LM13a -GGSIKSLVP		593.4095
LM13a -VLP / -PIV / -LVP		1122.6906	LM13a -IVLPGIGGSI		525.3398
LM13a -VLPG		1065.6654	LM13a -IGGSIKSLVP		480.3174
LM13a -LVPI / -IVLP		1009.6015	LM13a -IGGSIKSLVPI		367.2330
LM13a -IVLPG / -VLPGI		952.5800	PVL / PLV / LVI / VIP		310.2119
LM13a -IVLPG / -VLPGI	-CO	924.5857	IP / PL		211.1430
LM13a -KSLVP		907.5642			

LM13b

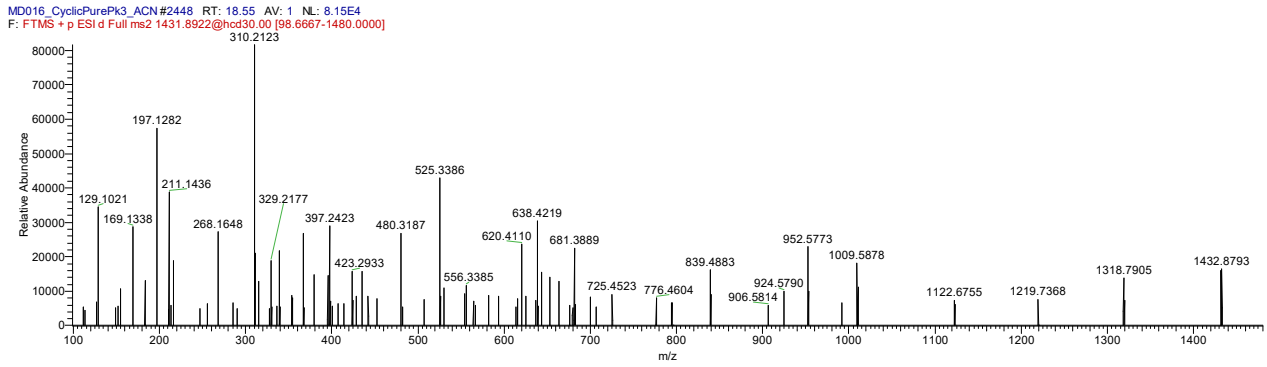


Figure S19: MS^2 fragmentation pattern of cyclic peptide LM13b.

Ion	Additional	Observed m/z	Ion	Additional	Observed m/z
LM13a -I / -L		1318.7905	LM13a -IVLPGIGGS	$-H_2O$	620.4110
LM13a -VL / -IV / -LV		1219.7368	LM13a -IVLPGIGGSI		525.3386
LM13a -VLP / -PIV / -LVP		1122.6755	LM13a -IGGSIKSLVP		480.3187
LM13a -LVPI / -IVLP		1009.5878	IPVL / LVIP / PLVI		423.2933
LM13a -IVLPG / -VLPGI		952.5773	PVLS		397.2423
LM13a -IVLPG / -VLPGI	-CO	924.5790	LSK / SKI / KIS		329.2177
LM13a -IVLPGI		839.4883	PVL / PLV / LVI / VIP		310.2123
LM13a -IKSLVP	$-H_2O$	776.4604	GPL / IGP		268.1648
LM13a -IVLPGIGG		725.4523	IP / PL		211.1430
LM13a -IKSLVPI		681.3889	PV		197.1282
LM13a -IVLPGIGGS		638.4219	PV	-CO	169.1338
			K		129.1021