Supporting Information for:

X-ray Crystallographic Structures of Trimers and Higher-Order Oligomeric Assemblies of a Peptide Derived from $A\beta_{17-36}$.

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Materials and Methods

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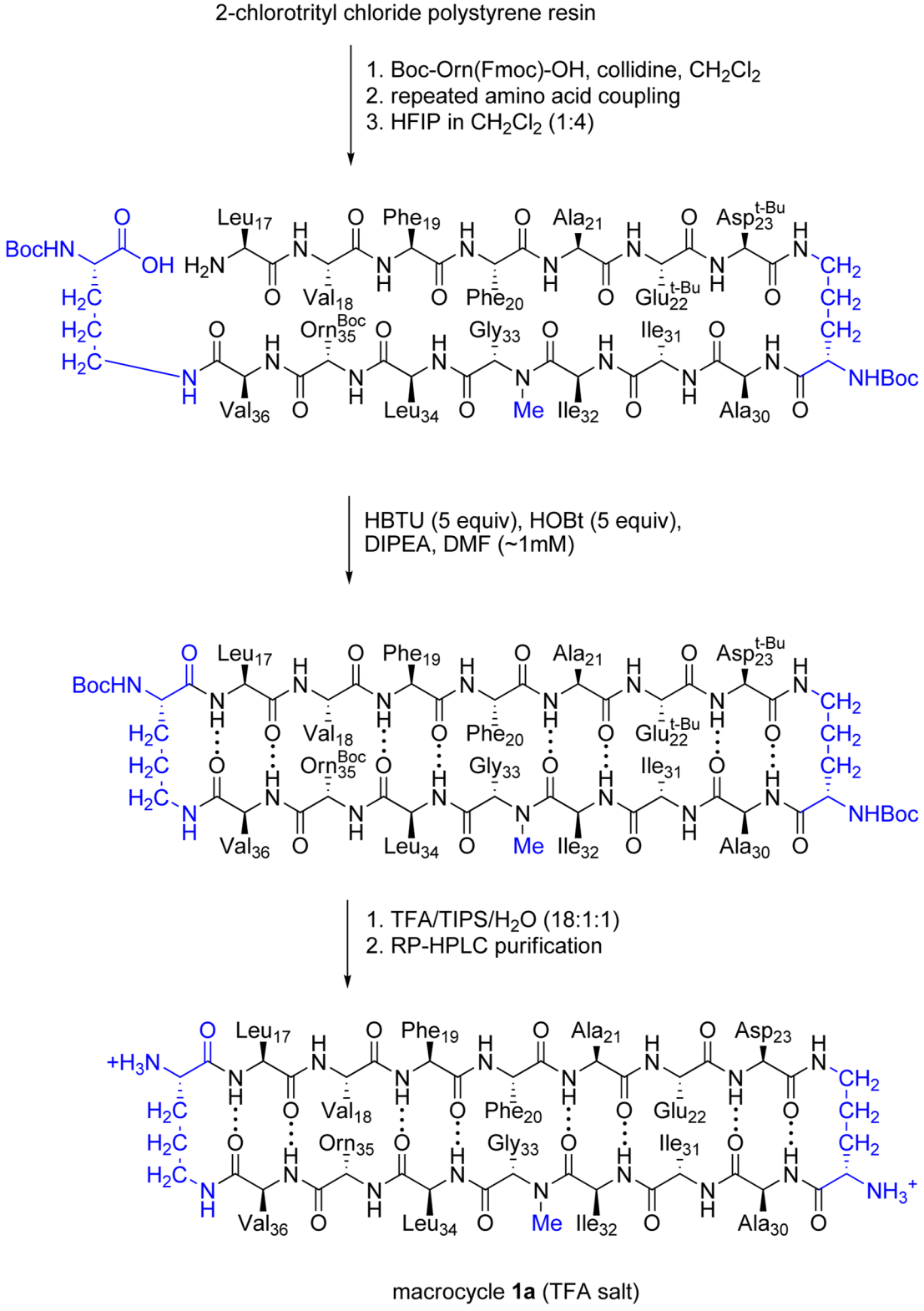
Materials and Methods

Scheme S1. Synthesis of peptide **1a**.



*Synthesis of peptides **1** and **2**. Representative synthesis of peptide **1a**.*

a. *Loading of the resin:* 2-Chlorotrityl chloride resin (300 mg, 1.2 mmol/g) was added to a Bio-Rad Poly-Prep chromatography column (10 mL, 0.8×4.0 cm). The resin was suspended in dry CH_2Cl_2 (10 mL) and allowed to swell for 30 min. The solution was drained from the resin and a solution of Boc-Orn(Fmoc)-OH (0.50 equiv., 82 mg, 0.18 mmol) in 20% 2,4,6-collidine in dry CH_2Cl_2 (5 mL) was added immediately and the mixture was gently agitated for 12 h. The solution was then drained and a mixture of CH_2Cl_2/MeOH/DIPEA (17:2:1, 10 mL) was added immediately. The mixture was gently agitated for 1 h to cap the unreacted 2-chlorotrityl chloride sites. The resin was then washed with dry CH_2Cl_2 (2x) and dried by passing nitrogen through the vessel. In the synthesis of peptide **1a**, the resin loading was determined to be 0.14 mmol [0.46 mmol/g, 77% based on Boc-Orn(Fmoc)-OH] by UV analysis of the Fmoc cleavage product. Loadings of 0.12–0.15 mmol [70–80%, based on Boc-Orn(Fmoc)-OH] were typically observed in various repetitions of this procedure associated with the syntheses of peptides **1** and **2**.

b. *Peptide Coupling:* The PS-2-chlorotrityl-Orn(Fmoc)-Boc generated from the previous step was transferred to a solid-phase peptide synthesizer reaction vessel and submitted to cycles of automated peptide coupling with Fmoc-protected amino acid building blocks. The linear peptide was synthesized from the C-terminus to the N-terminus. Each coupling consisted of i. Fmoc-deprotection with 20% piperidine in DMF for 3 min, ii. washing with DMF (3x), iii. coupling of the amino acid (0.56 mmol, 4 equiv.) in the presence of HCTU (224 mg, 0.56 mmol, 4 equiv.), and iv. washing with DMF (6x). Each amino acid coupling step took 20 min for all the residues of peptide **1a**. For peptides **1b** and **2b**, the phenylalanine and 4-iodophenylalanine residues after the *N*-methyl-L-phenylalanine were double coupled (0.56

mmol, 4 equiv.) and allowed to react for 1 h per coupling with HATU (4 equiv.) and HOAt (4 equiv.). Other residues of peptides **1b** and **2b** were coupled as described previously. After coupling of the last amino acid, the terminal Fmoc group was removed with 20% piperidine in DMF. The resin was transferred from the reaction vessel of the peptide synthesizer to a Bio-Rad Poly-Prep chromatography column.

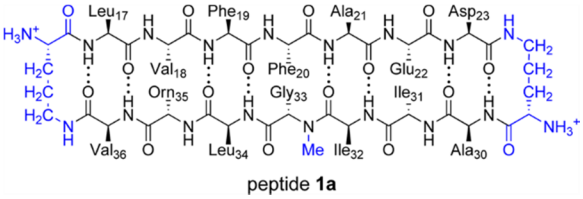
c. *Cleavage of the Peptide from the Resin:* The linear peptide was cleaved from the resin by agitating the resin for 1 hr with a solution of hexafluoroisopropanol (HFIP) in CH_2Cl_2 (1:4, 5 mL).[1] The suspension was filtered and the filtrate was collected in a 250 mL round-bottomed flask. The resin was washed with additional HFIP in CH_2Cl_2 (1:4, 5 mL) and then with CH_2Cl_2 (2×10 mL). The combined filtrates were concentrated by rotary evaporation to give a white solid. The white solid was further dried by vacuum pump to afford the crude protected linear peptide, which was cyclized without further purification.

d. *Cyclization of the Linear Peptide:* Crude protected linear peptide was dissolved in dry DMF (125 mL). HOBt (95 mg, 0.70 mmol, 5 equiv.) and HBTU (264 mg, 0.70 mmol, 5 equiv.) were added to the solution. The reaction mixture was then stirred under nitrogen for 20 min. DIPEA (0.3 mL, 1.7 mmol, 12 equiv.) was added to the solution and the mixture was stirred under nitrogen for 24 h. The mixture was concentrated under reduced pressure to afford crude protected cyclic peptide.

1. Bollhagen, R.; Schmiedberger, M.; Barlosb, K.; Grell, E. *J. Chem. Soc., Chem. Commun*., **1994**, 2559-2560.

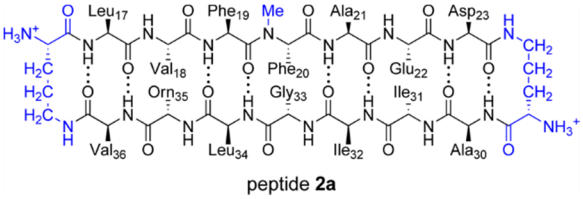
e. *Global Deprotection and Purification of the Cyclic Peptide:* Protected cyclic peptide was dissolved in TFA/triisopropylsilane (TIPS)/H_2O (18:1:1, 10 mL) in a 250 mL round-bottomed flask equipped with a nitrogen-inlet adaptor. The solution was stirred for 1.5 h. The reaction mixture was then concentrated by rotary evaporation under reduced pressure to afford the deprotected cyclic peptide as a yellow oil. The oil was dissolved in H_2O and acetonitrile (4:1, 5 mL) and the solution was filtered through a 0.20 μm syringe filter and purified by reversed-phase HPLC (gradient elution with 20–50% CH_3CN over 40 min). The pure fractions were lyophilized to afford 53 mg of the cyclic deprotected peptide **1a**. The syntheses of peptides **1b**, **2a**, and **2b** afforded 64, 67, and 120 mg respectively.

*Optimized crystallization conditions for peptides **1a**, **1b**, **2a**, and **2b**.*



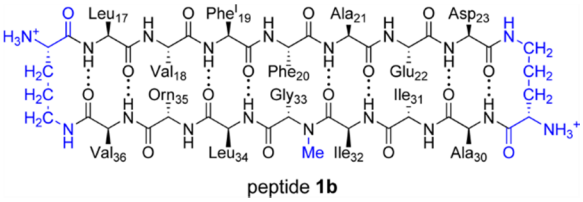
peptide **1a**

peptide **1a**	
Buffer	0.1 M HEPES, pH 6.75
Jeffamine M-600 pH 7.0	31% v/v
Temperature	23°C
Crystallization time	<24 hours
PDB entry code	4NTR



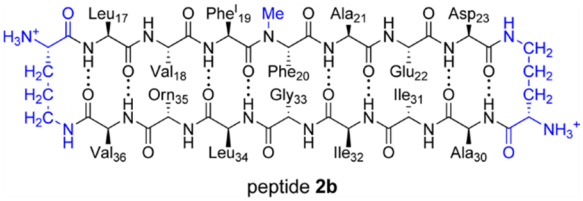
peptide **2a**

peptide **2a**	
Buffer	0.1 M HEPES, pH 6.5
Jeffamine M-600 pH 7.0	24% v/v
Temperature	23°C
Crystallization time	<24 hours
PDB entry code	4NW9



peptide **1b**

peptide **1b**	
Buffer	0.1 M HEPES, pH 6.5
Jeffamine M-600 pH 7.0	25% v/v
Temperature	23°C
Crystallization time	<24 hours
PDB entry code	4NTP



peptide **2b**

peptide **2b**	
Buffer	0.1 M HEPES, pH 7.5
Jeffamine M-600 pH 7.0	29% v/v
Temperature	23°C
Crystallization time	<24 hours
PDB entry code	4NW8

Crystallization procedure:

Initial crystallization conditions were determined using the hanging-drop vapor-diffusion method. Crystallization was performed in a 96-well format, with each well containing 100 µL of a solution from a Hampton 96-well screening kit. Three kits were used — Crystal Screen, Index, and Peg/Ion — for a total of 288 experiments (three 96-well plates). Hanging-drops were made by combining 300 nL of peptide **1b** (solution of 10 mg/mL in18 MΩ water) and 300 nL of the well solution using a TTP LabTech Mosquito nanodisperse instrument. Crystal grew rapidly (<24 h) in a solution of 0.1 M 2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid (HEPES) buffer at pH 7.0 and Jeffamine M-600 at pH 7.0 (30% v/v).

We optimized crystallization conditions using a 4x6 matrix Hampton VDX 24-well plate. We varied the HEPES buffer pH in each row by ±0.5 pH units (6.5, 7.0, 7.5, and 8.0) and the pH 7.0 Jeffamine M-600 concentration in each column by ±2% (24%, 26%, 28%, 30%, 32%, and 34% v/v). For the first well in the 4x6 matrix we combined 100 μL of 1 M HEPES pH 6.5, 480 μL of a 50% solution (v/v) of pH 7.0 Jeffamine M-600, and 420 μL of 18 MΩ water. [The 50% pH 7.0 Jeffamine M-600 solution was prepared by combining 200 mL of pH 10.0 Jeffamine M-600 and 200 mL of 18 MΩ water, titrating with hydrochloric acid to pH 7.0, and filtering through a 0.2 μm syringe filter.] The other wells were prepared in analogous fashion, by combining 100 μL of HEPES buffer, pH 7.0 Jeffamine M-600, and 18 MΩ water for a total volume of 1 mL.

Three hanging-drops were prepared per borosilicate glass slide by combining a solution of peptides **1** or **2** (1 μL, 10 mg/mL) and the well solution (1 μL) in a ratio of 1:1, 2:1, and 1:2. Slides were inverted and pressed firmly against the silicone grease surrounding each well. Large crystals, (0.3 – 0.4 mm) grew in under 24 hours. Crystallization conditions were further optimized using smaller variations in HEPES buffer pH (±0.25 pH units) and Jeffamine M-600 concentrations (±1%). Crystal were harvested with a nylon loop attached to a copper or steel pin and flash frozen in liquid nitrogen prior to data collection. The optimized crystallization conditions for peptides **1a**, **1b**, **2a**, and **2b** are summarized above.

Data Collection and Processing

Diffraction data for peptides **1a** and **2a** were collected at Lawrence Berkeley National Laboratory (Berkeley, California) on synchrotron beamline 8.2.2 at 1.0 Å wavelength with 0.5° oscillation and a detector distance of 220 mm.[2] Diffraction data were scaled and merged using

2. The Berkeley Center for Structural Biology is supported in part by the National Institutes of Health, National Institute of General Medical Sciences, and the Howard Hughes Medical

XDS.[3] Electron density maps were generated by isomorphous replacement of coordinates from peptide **1b** using Phaser in software suite Phenix 1.8.4.[4] Molecular manipulations of the models were performed with Coot.[5] Coordinates were refined with phenix.refine.

Diffraction data for peptides **1b** and **2b** were collected on a Rigaku Micromax-007HF X-ray diffractometer with a rotating copper anode at 1.54 Å wavelength with 0.5° oscillation. Diffraction data were collected using CrystalClear. Diffraction data were scaled and merged using XDS.[1] Coordinates for the anomalous signals were determined by HySS in the Phenix software suite.[2] Electron density maps were generated using anomalous coordinates determined by HySS as initial positions in Autosol. Molecular manipulations of the models were performed with Coot. Coordinates were refined with phenix.refine.

Modeling of Ac-Aβ$_{17-36}$-NHMe trimer using replica-exchange molecular dynamics (REMD).

Coordinates for REMD were generated from the X-ray crystallographic coordinates of peptide **1a**. The trimer was edited in PyMOL as follows: The δ-linked ornithine turn units were removed. Aβ residues Val$_{24}$, Gly$_{25}$, Ser$_{26}$, Gln$_{27}$, Lys$_{28}$, and Gly$_{29}$ were added to link Asp$_{23}$ and Ala$_{30}$. Orn$_{35}$ was mutated to Met$_{35}$. The N-terminus was patched as an acetylated amide (ACE) and the C-terminus was patched as a methylamide (CT3) in VMD. The requisite .psf file was

Institute. The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
3. Kabsch, W. *Acta Cryst.*, **2010**, D66, 125-132.
4. Adams, P. D.; Afonine, P. V.; Bunkóczi, G.; Chen, V. B.; Davis, I. W.; Echols, N.; Headd, J. J.; Hung, L.-W.; Kapral, G. J.; Grosse-Kunstleve, R. W.; McCoy, A. J.; Moriarty, N. W.; Oeffner, R.; Read, R. J.; Richardson, D. C.; Richardson, J. S.; Terwilliger, T. C.; Zwart., P. H. *Acta Cryst.*, **2010**, D66, 213-221.
5. Emsley, P.; Lohkamp, B.; Scott, W. G.; Cowtan, K. *Acta. Cryst.*, **2010**, D66, 486-501.

generated using the autopsf plugin in VMD.[6] The coordinates for the main chains of residues Leu_{17}-Asp_{23} and Ala_{30}-Val_{36} were frozen during the simulation. Residues Val_{24}-Gly_{29} and all side chains were allowed to move freely. REMD simulations were run in NAMD with the CHARMM22 force field and generalized Born implicit solvent (GBIS) on 32 replicas with a temperature range of 300K-800K for 20 ns.[7] The coordinates for the 20 lowest energy conformations were selected.

6. Humphrey, W.; Dalke, A.; Schulten, K. *J. Molec. Graphics*, **1996**, *14.1*, 33-38.
7. Phillips, J. C.; Braun, R.; Wang, W.; Gumbart, J.; Tajkhorshid, E.; Villa, E.; Chipot, C.; Skeel, R. D.; Kale, L.; Schulten, K. *Journal of Computational Chemistry*, **2005**, *26*,1781-1802.

Table S1. Crystallographic Data Reported for Collection and Refinement of Peptides **1a**, **1b**, **2a**, and **2b**.

	peptide **1a**	peptide **1b**	peptide **2a**	peptide **2b**
Space group	R3:H	R3:H	$P3_221$	$P3_221$
***a,b,c* (Å)**	68 68 169.26	68.18 68.18 170.43	68.22 68.22 92.99	68.68 68.68 93.84
α, β, γ (deg)	90 90 120	90 90 120	90 90 120	90 90 120
Wavelength (Å)	1.0	1.54	1.0	1.54
Peptides per asymmetric unit	16	16	12	12
Resolution (Å)	34.36 - 1.7 (1.761 - 1.700)	34.09 - 1.987 (2.058 - 1.987)	36.54 - 1.655 (1.713 - 1.654)	29.74 - 2.023 (2.095 - 2.023)
Total reflections	98412 (9014)	472254 (13643)	173645 (14559)	121088 (4284)
Unique reflections	31708 (3062)	20197 (1852)	29970 (2640)	16770 (1268)
Multiplicity	3.1 (2.9)	23.4 (7.4)	5.8 (5.5)	7.2 (3.4)
Completeness (%)	98.74 (94.80)	99.11 (91.10)	98.42 (88.35)	97.38 (75.21)
Mean I/σ	12.63 (2.25)	22.24 (3.43)	13.78 (1.02)	28.82 (3.41)
Wilson B-factor	24.24	23.13	31.33	25.70
R_{merge}	0.04665 (0.5536)	0.1366 (0.487)	0.05206 (1.478)	0.1246 (0.3187)
$R_{measure}$	0.05651	0.139	0.0573	0.1334
CC½	0.998 (0.807)	1 (0.891)	0.999 (0.53)	0.998 (0.906)
CC*	0.999 (0.945)	1 (0.971)	1 (0.833)	1 (0.975)
		Refinement		
R_{work}	0.2002	0.2068	0.1886	0.1952
R_{free}	0.2262	0.2461	0.2095	0.2372
Number of non-hydrogen atoms	2239	2294	1740	1703
macromolecules	1984	2000	1488	1500
Ligands	11	7	5	4
Waters	244	287	247	199
RMS_{bonds}	0.008	0.008	0.012	0.007
RMS_{angles}	1.20	1.27	1.63	1.14
Ramachandran favored (%)	100	100	100	100
Ramachandran outliers (%)	0	0	0	0
Clashscore	0.71	2.62	5.72	4.14
Average B-factor	34.90	29.90	41.50	28.30
macromolecules	33.90	29.20	39.10	27.10
Ligands	60.20	53.20	64.30	43.70
Solvent	42.00	34.10	55.90	37.20

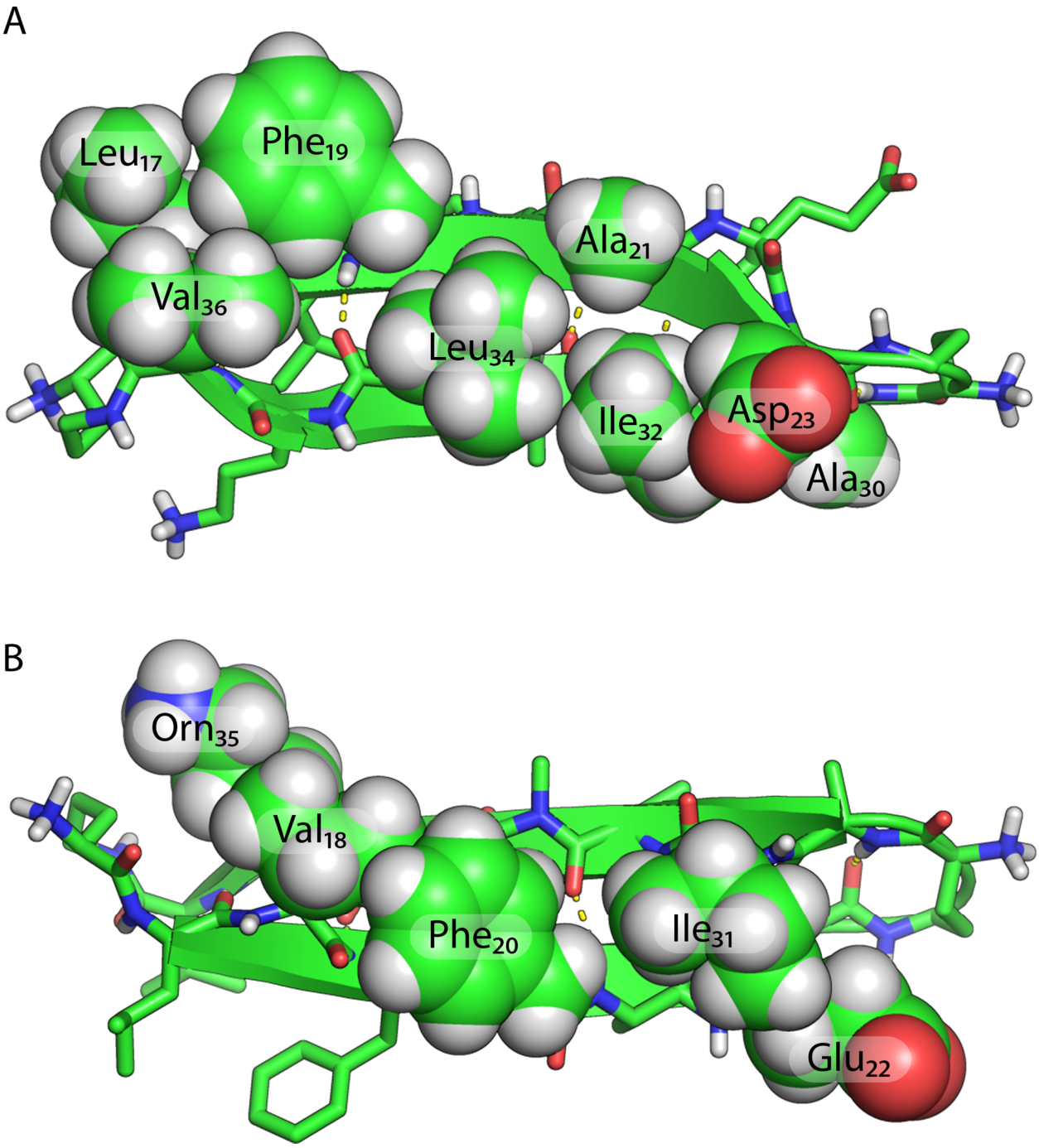


Figure S1. Contacts among side chains on the LFA (A) and VF (B) faces of peptide **1a**.

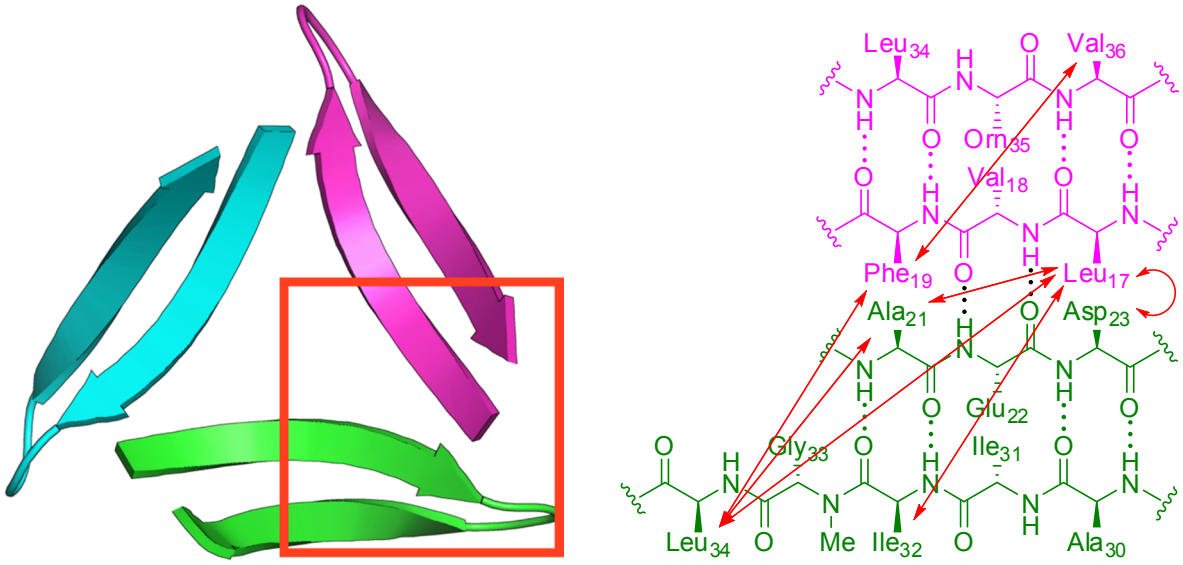


Figure S2. Important interstrand contacts at the corners of the trimer of peptide **1a**.

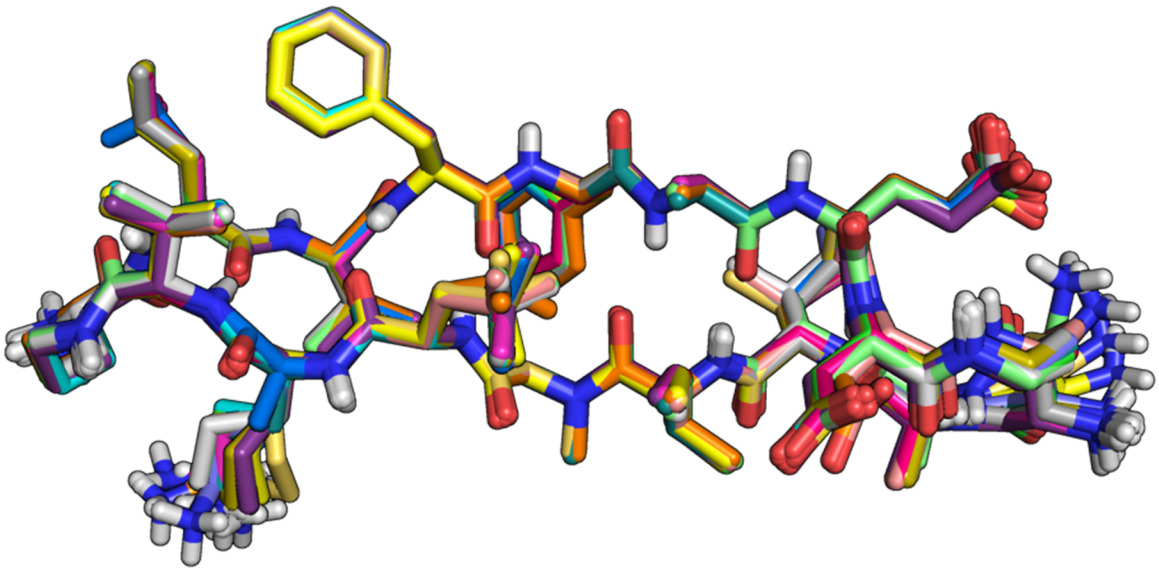


Figure S3. Overlay of the 16 β-hairpins in the asymmetric unit of the X-ray crystallographic structure of peptide **1a** (RMSD ≈ 0.2 Å).

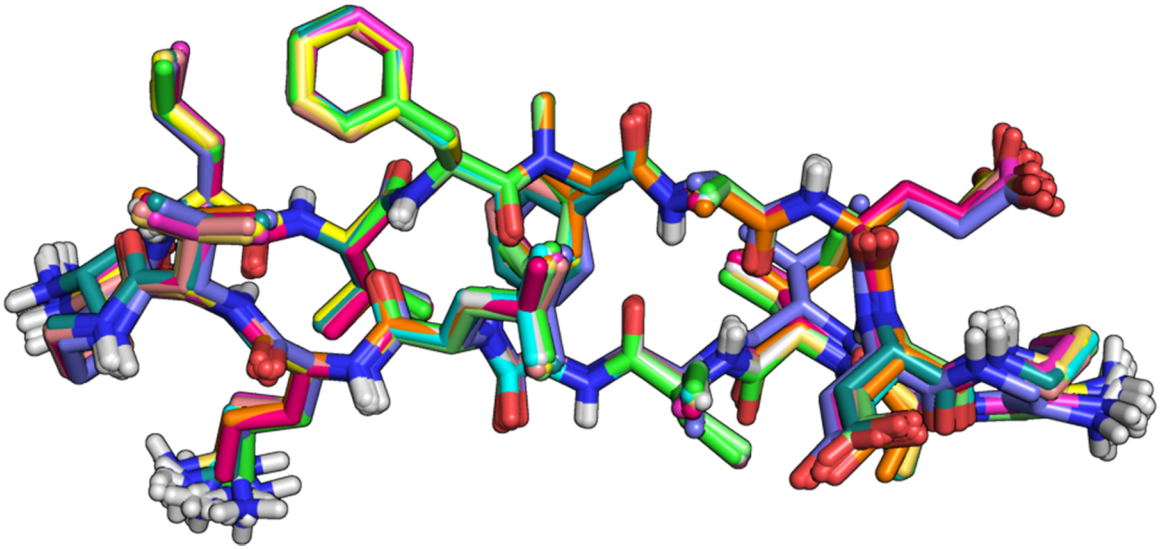
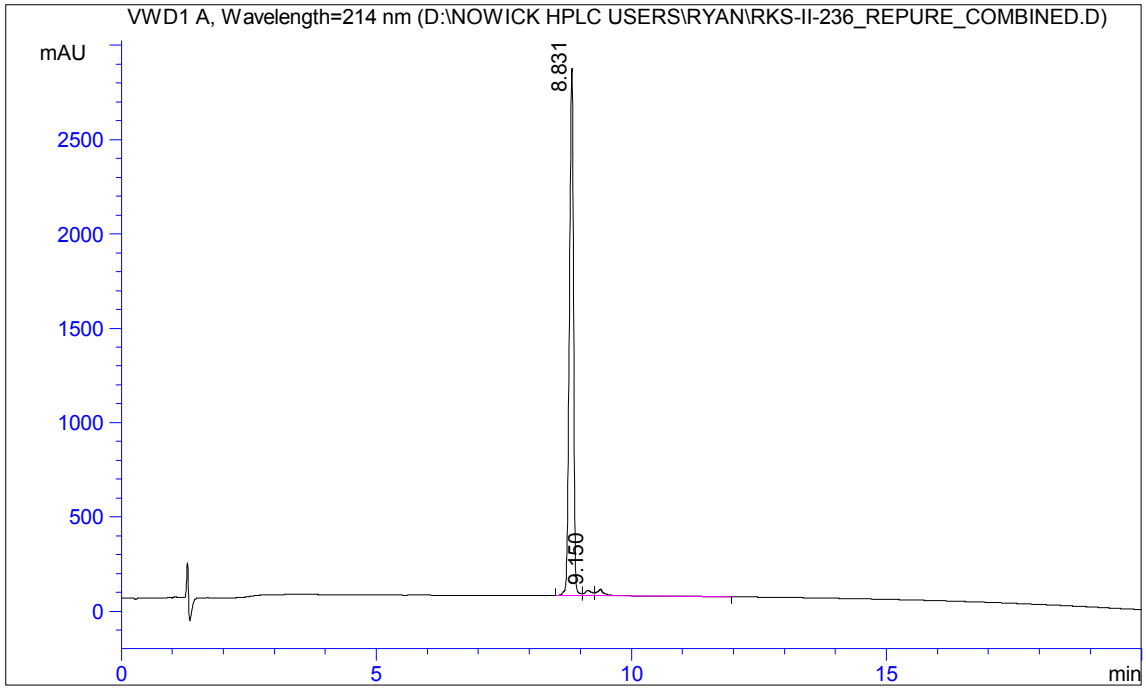


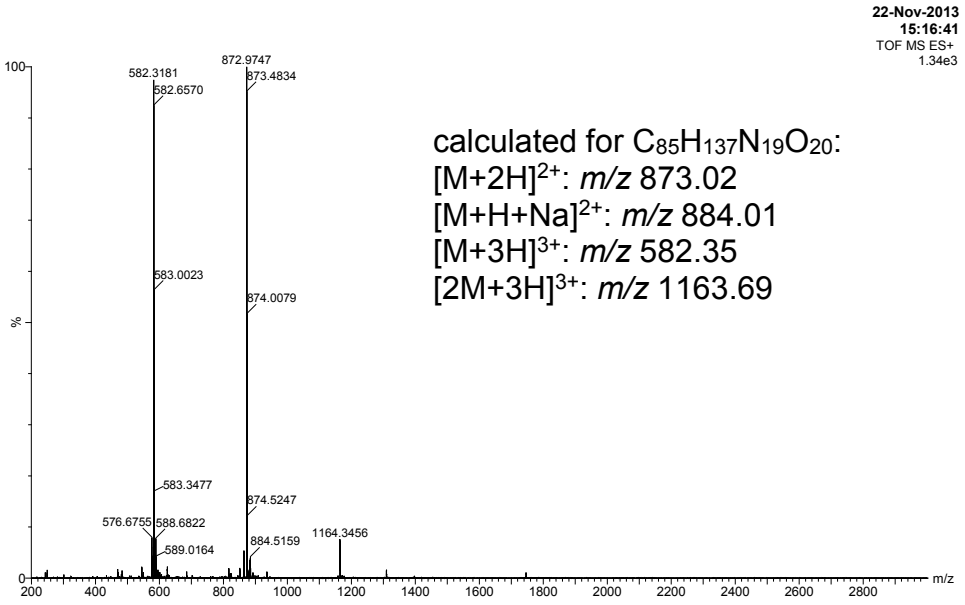
Figure S4. Overlay of the 12 β-hairpins in the asymmetric unit of the X-ray crystallographic structure of peptide **2a** (RMSD ≈ 0.3 Å).

HPLC and MS ESI+ TOF of peptide **1a**

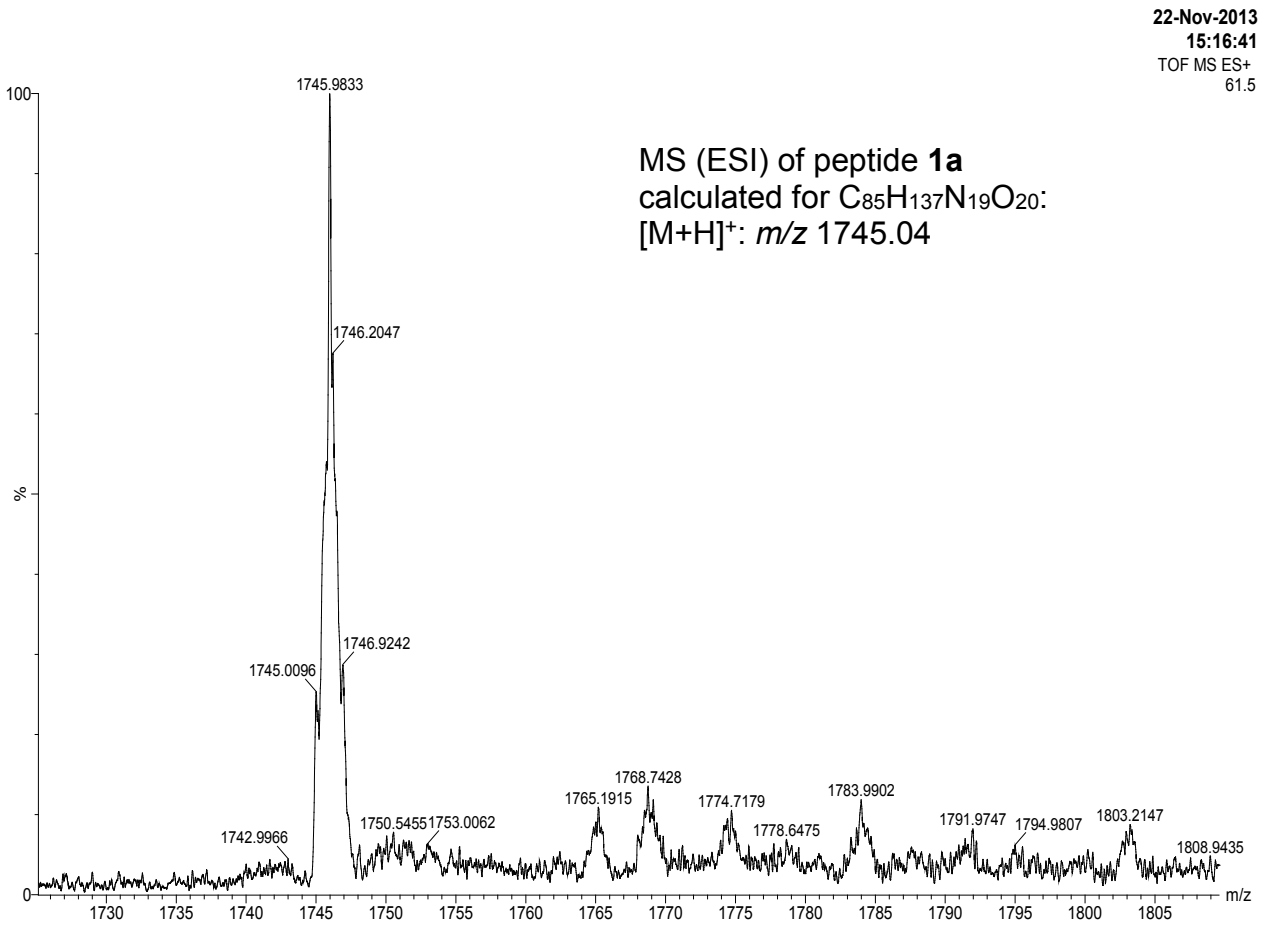


Signal 1:VWD1 A, Wavelength=214 nm

Peak #	RT [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	8.831	BV	0.089	15767.279	97.834	95.734
2	9.150	VV	0.139	268.146	0.966	1.628
3	9.394	VB	0.165	434.398	1.201	2.638



calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+2H]^{2+}$: *m/z* 873.02
$[M+H+Na]^{2+}$: *m/z* 884.01
$[M+3H]^{3+}$: *m/z* 582.35
$[2M+3H]^{3+}$: *m/z* 1163.69


22-Nov-2013
15:16:41
TOF MS ES+
61.5
MS (ESI) of peptide **1a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+H]^+$: *m/z* 1745.04
1745.9833
1746.2047
1746.9242
1745.0096
1742.9966
1750.5455
1753.0062
1765.1915
1768.7428
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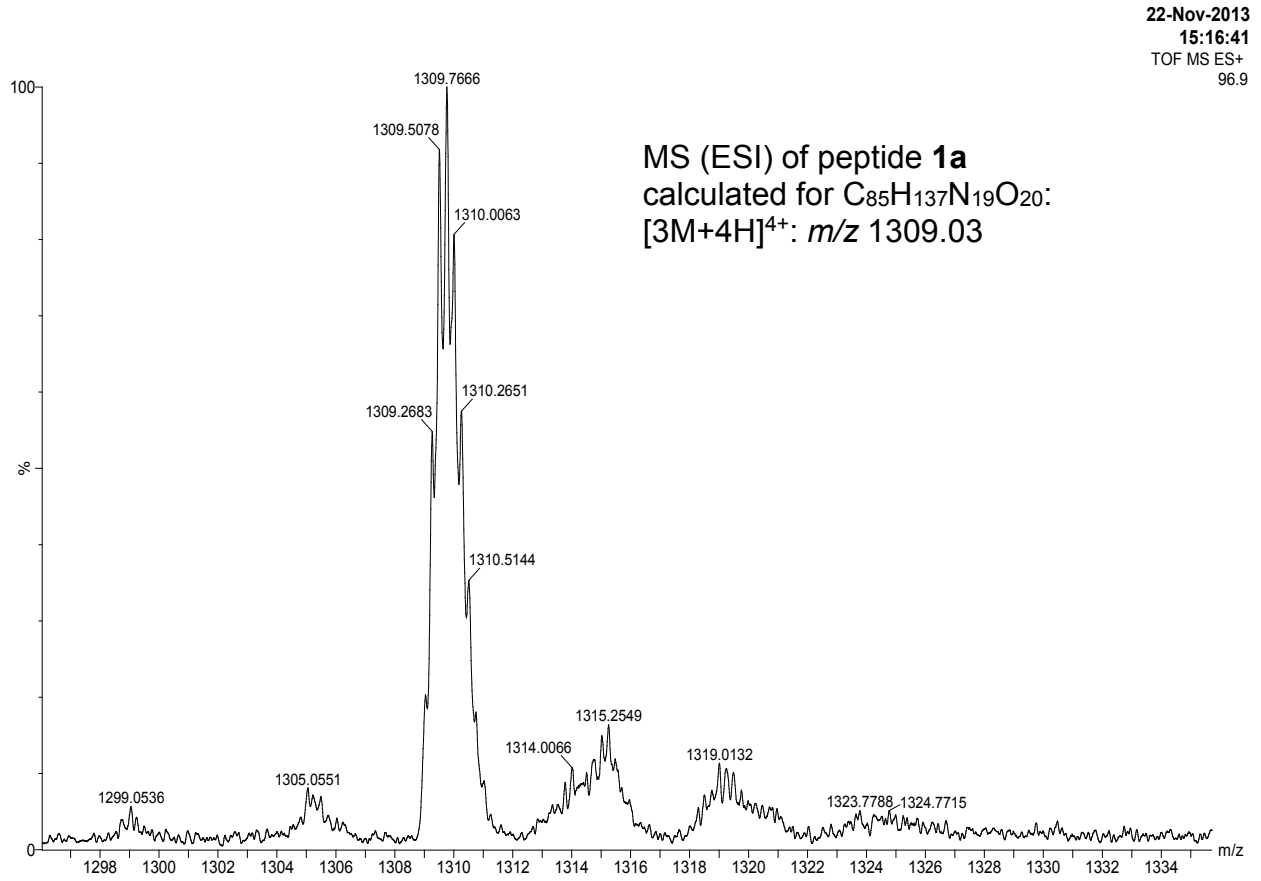
1808.9435
%
m/z


22-Nov-2013
15:16:41
TOF MS ES+
96.9
MS (ESI) of peptide **1a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[3M+4H]^{4+}$: *m/z* 1309.03
1309.7666
1309.5078
1310.0063
1310.2651
1309.2683
1310.5144
1315.2549
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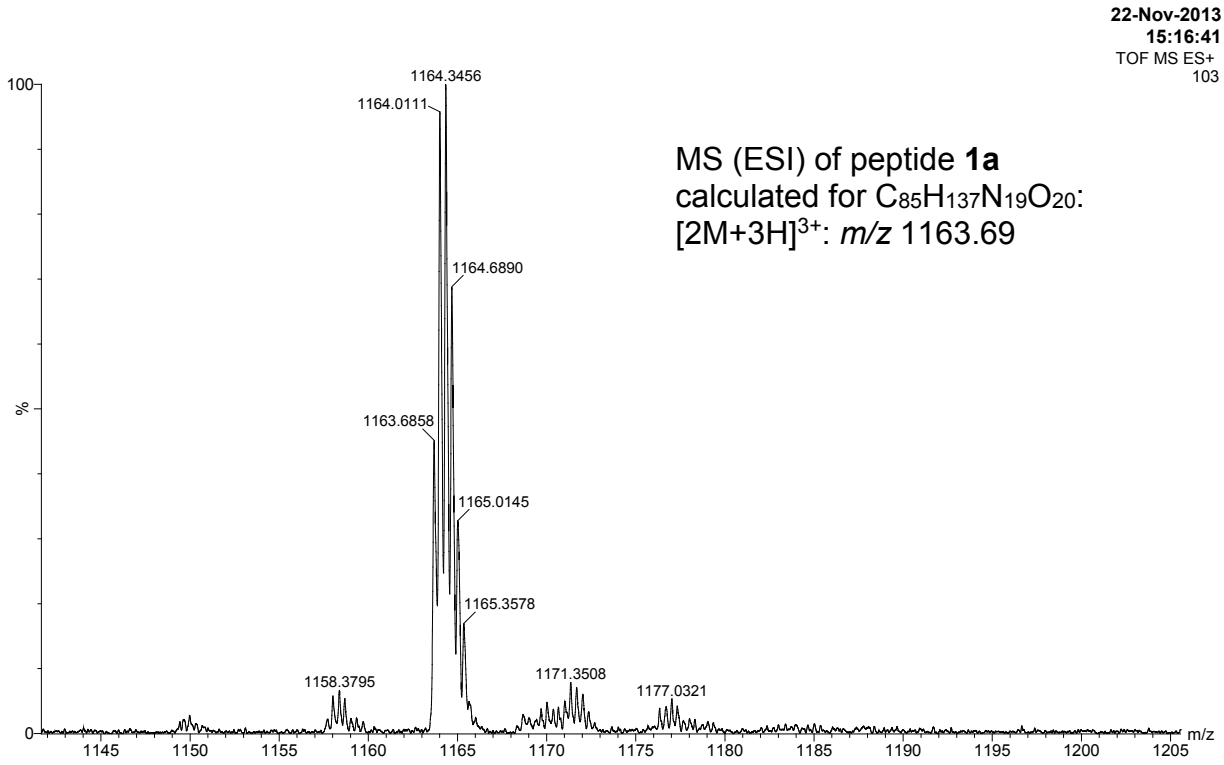
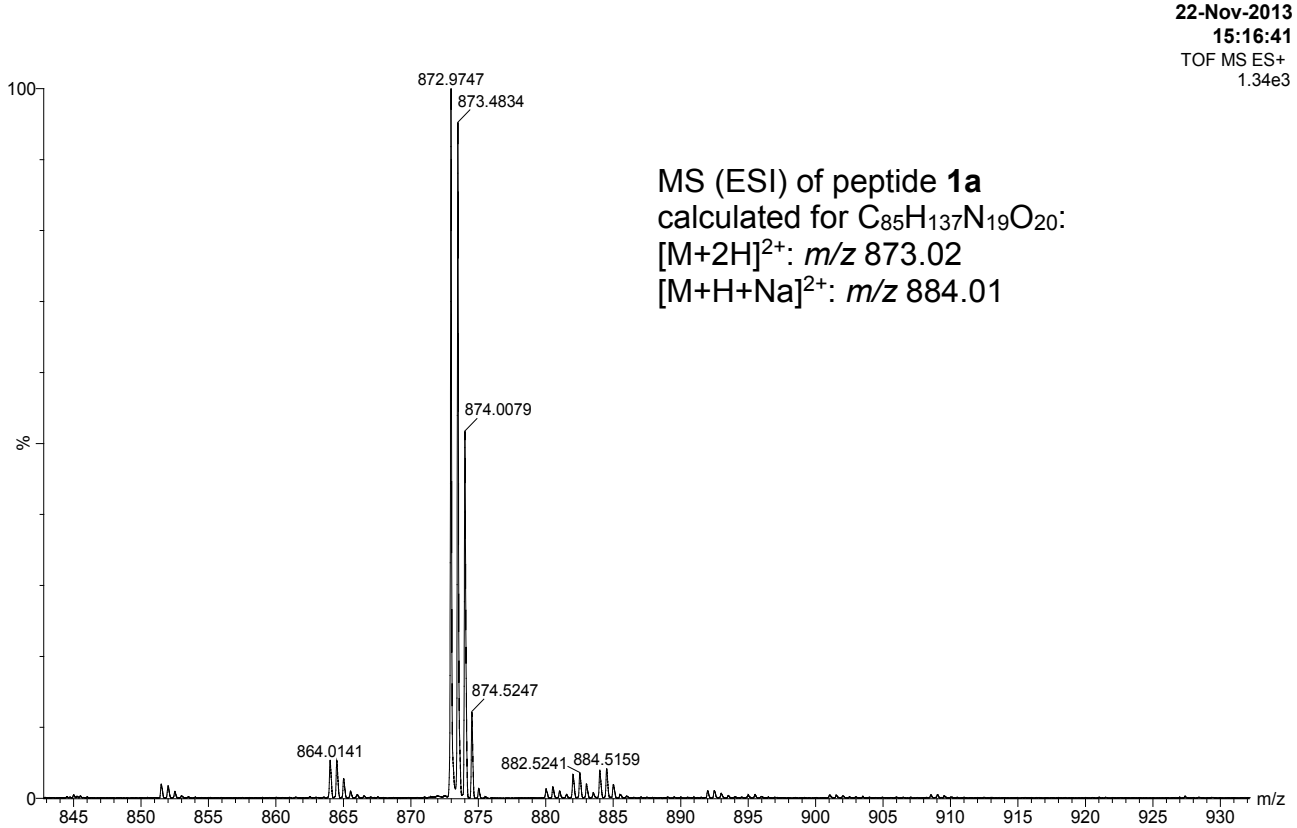
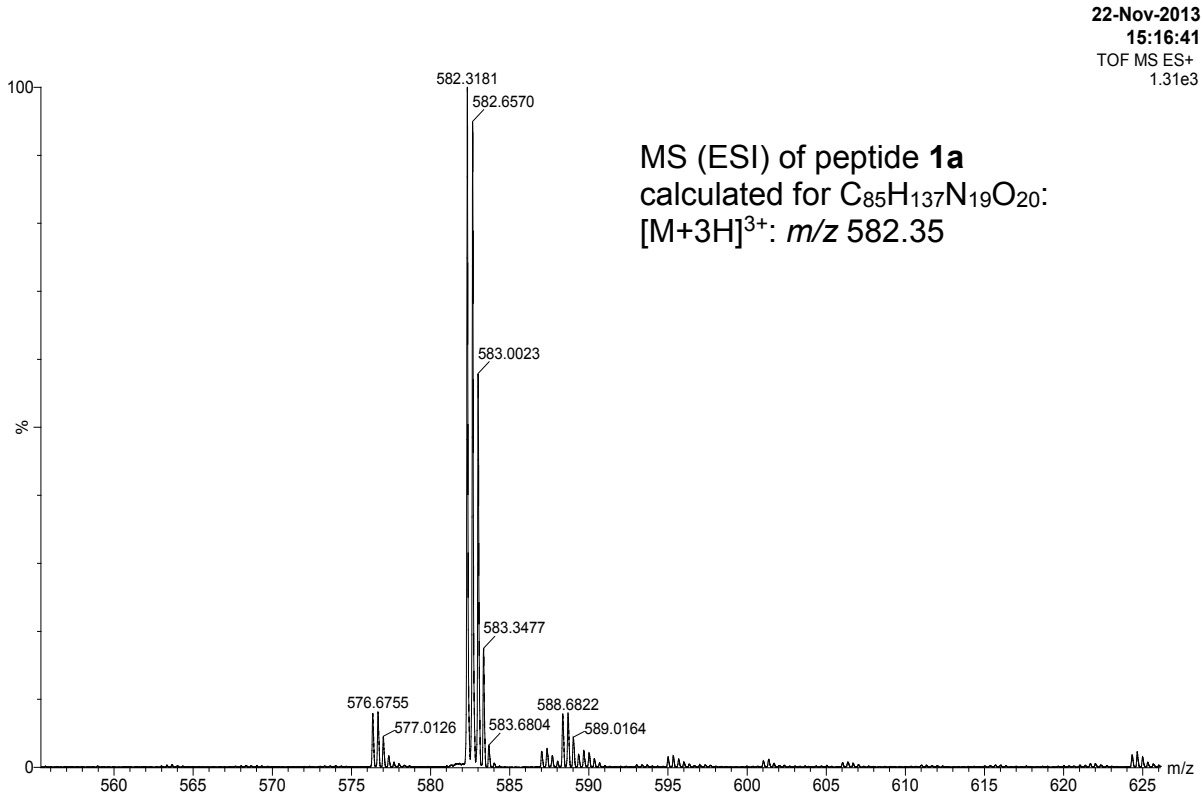
1324.7715
%
m/z



MS (ESI) of peptide **1a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[2M+3H]^{3+}$: *m/z* 1163.69

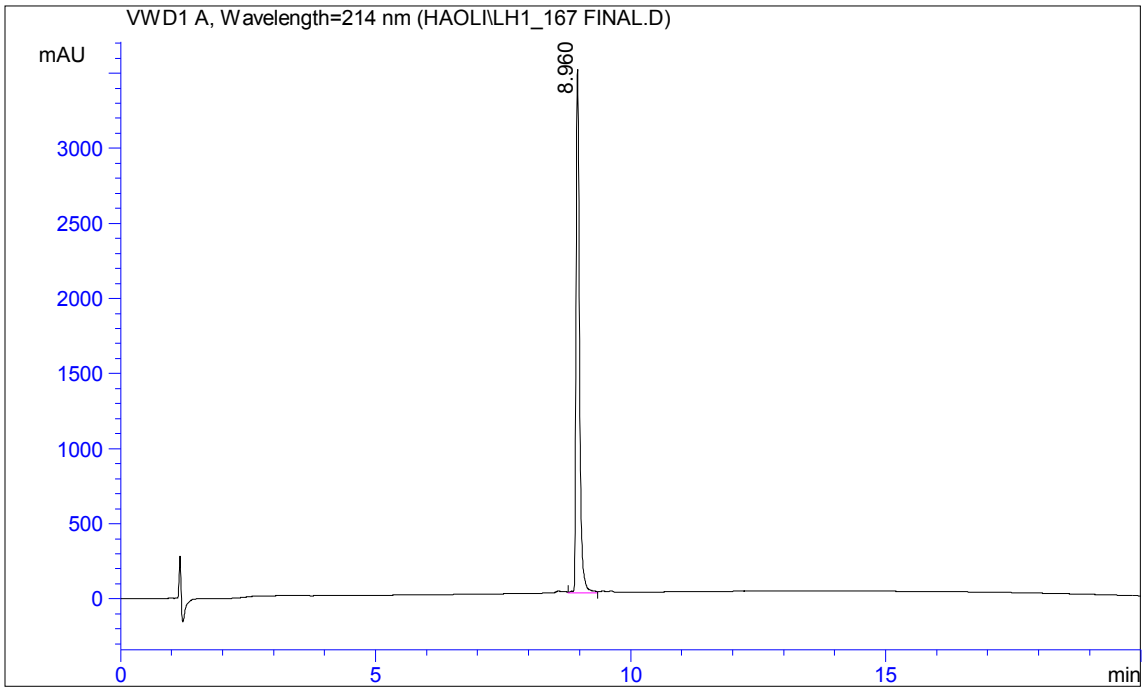


MS (ESI) of peptide **1a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+2H]^{2+}$: *m/z* 873.02
$[M+H+Na]^{2+}$: *m/z* 884.01



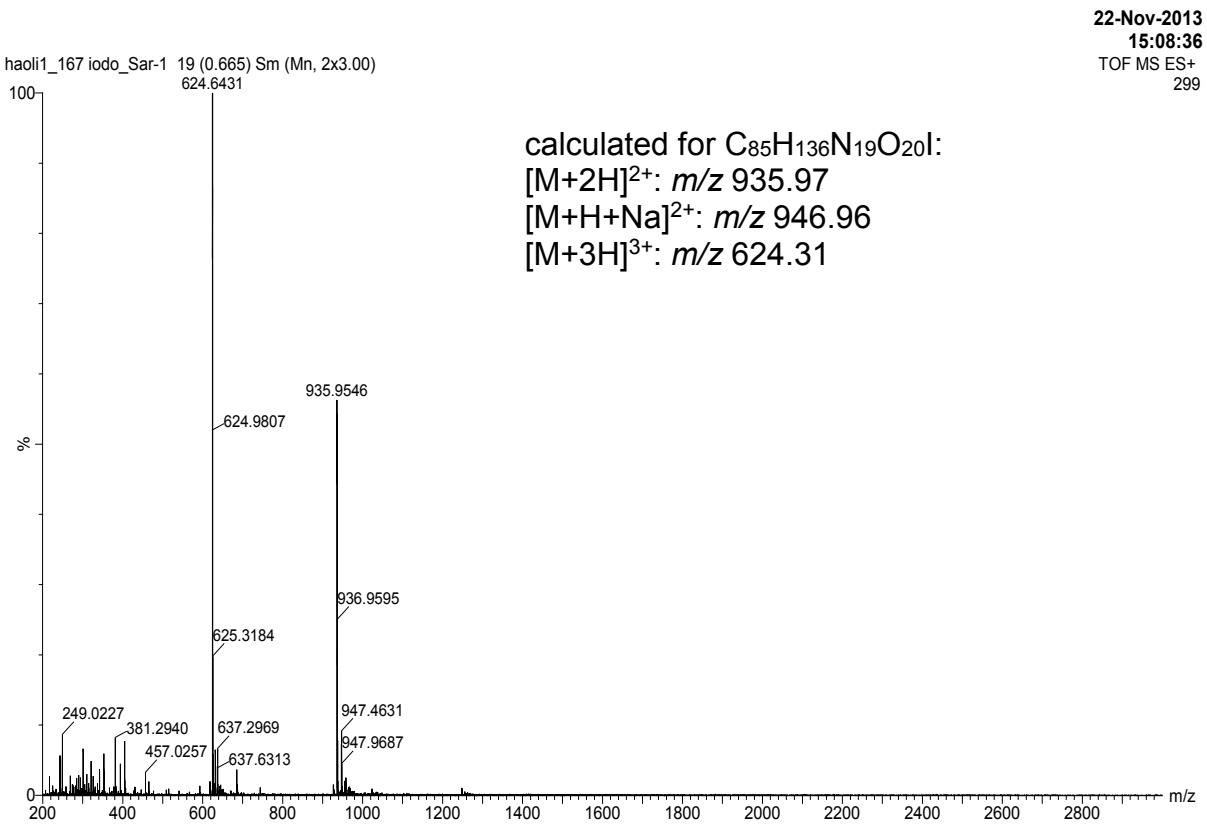
MS (ESI) of peptide **1a** calculated for $C_{85}H_{137}N_{19}O_{20}$: $[M+3H]^{3+}$: *m/z* 582.35

HPLC and MS ESI+ TOF of peptide **1b**

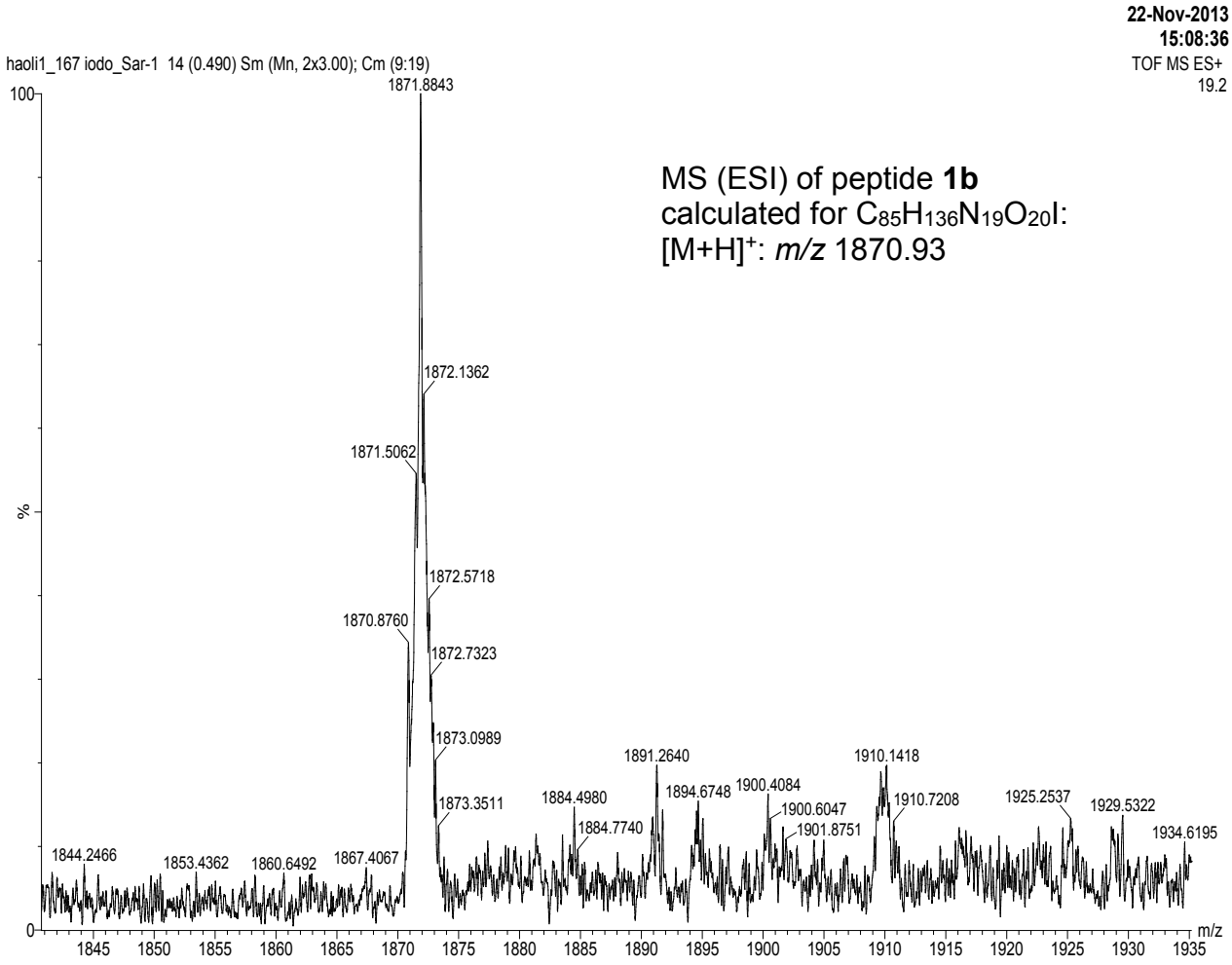


Signal 1:VWD1 A, Wavelength=214 nm

Peak #	RT [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	8.960	VV	0.072	16299.187	100.000	100.000



calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+2H]^{2+}$: *m/z* 935.97
$[M+H+Na]^{2+}$: *m/z* 946.96
$[M+3H]^{3+}$: *m/z* 624.31


22-Nov-2013
15:08:36
TOF MS ES+
19.2
haoli1_167 iodo_Sar-1 14 (0.490) Sm (Mn, 2x3.00); Cm (9:19)
MS (ESI) of peptide **1b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+H]^+$: *m/z* 1870.93
1871.8843
1872.1362
1871.5062
1872.5718
1870.8760
1872.7323
1873.0989
1873.3511
1891.2640
1910.1418
1884.4980
1894.6748
1900.4084
1900.6047
1910.7208
1925.2537
1929.5322
1884.7740
1901.8751
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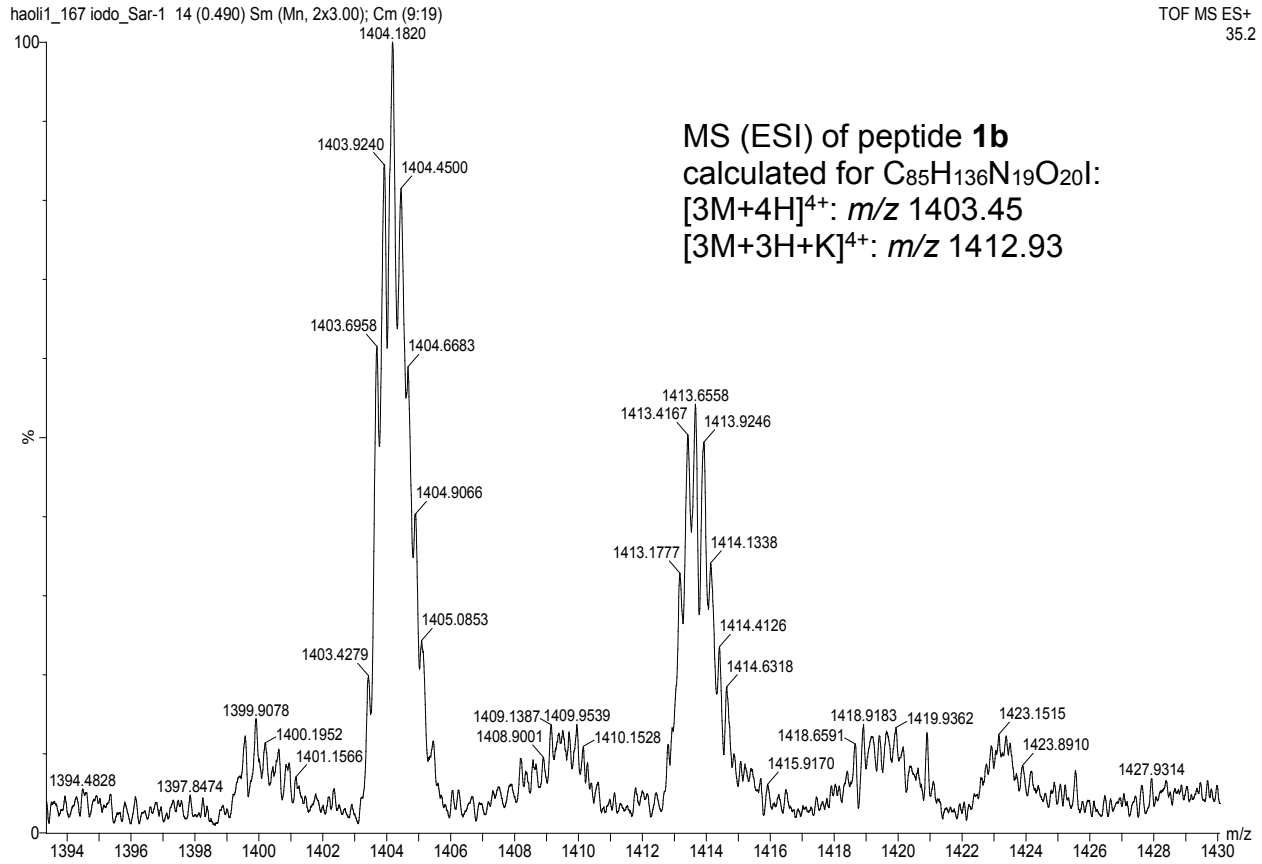
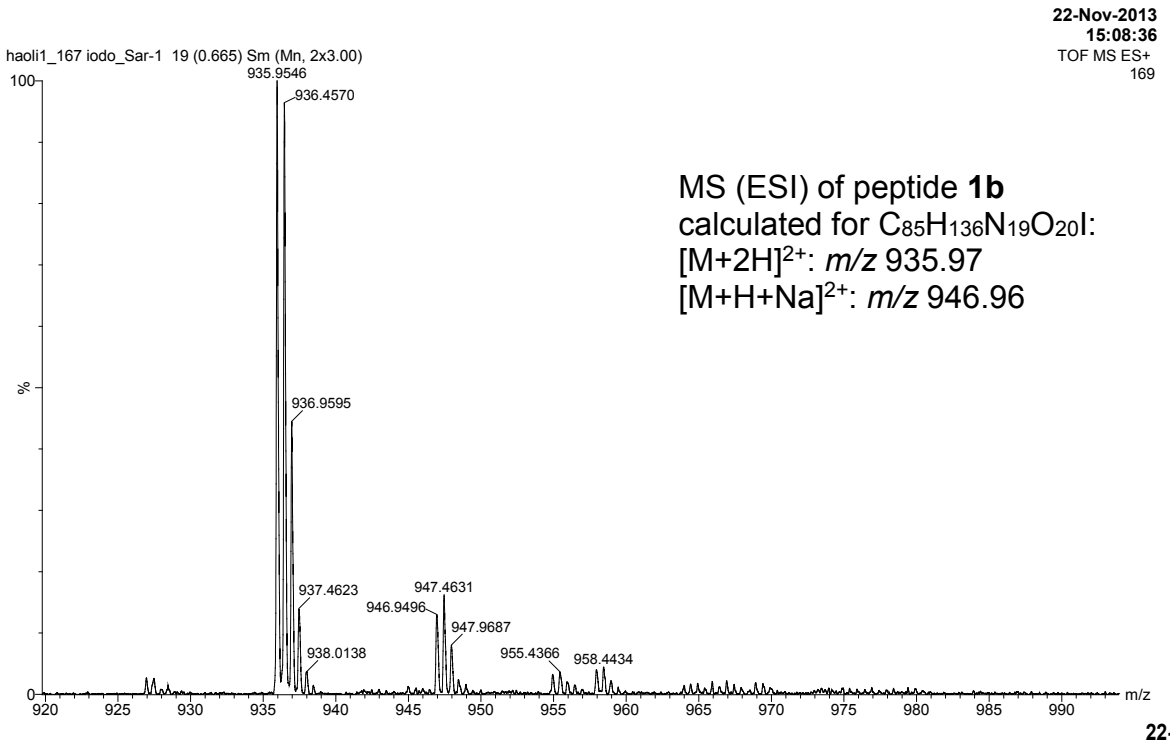
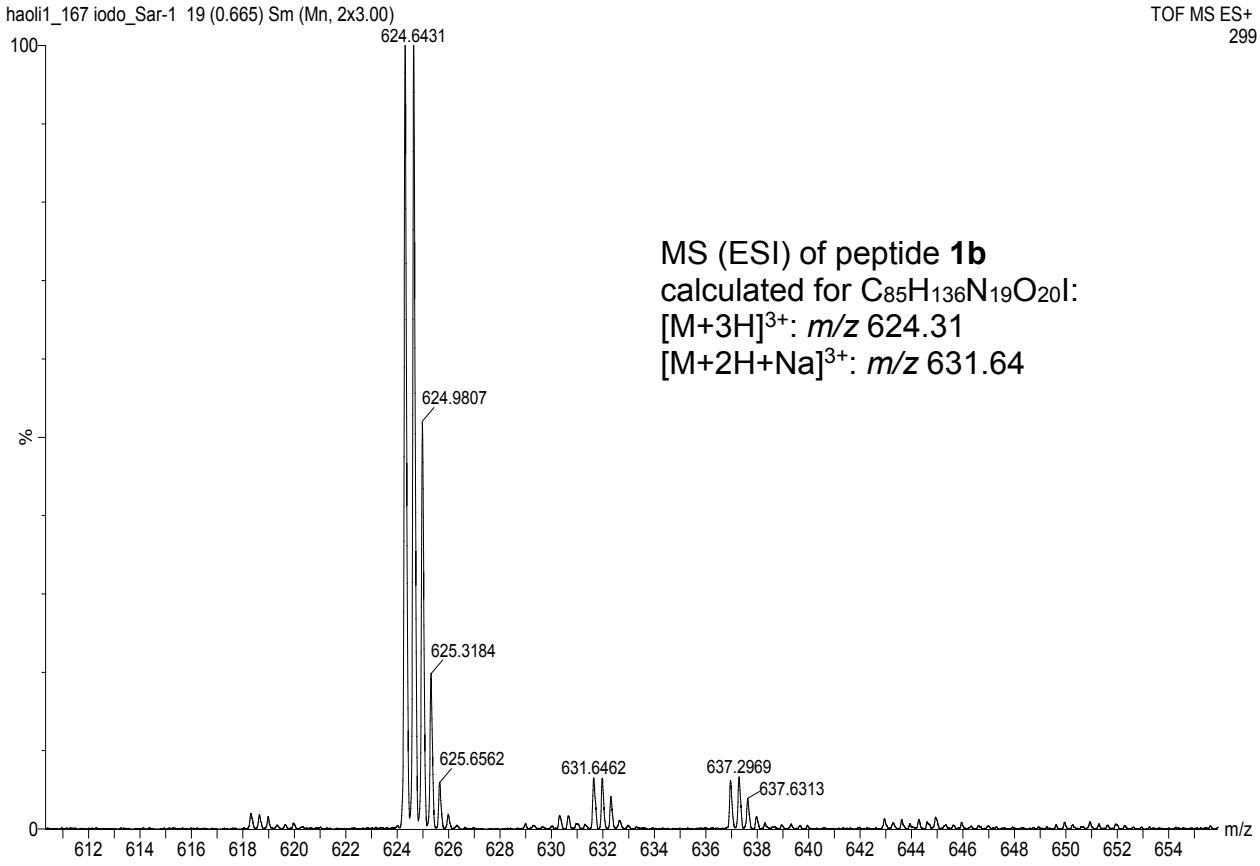
1860.6492
1867.4067
%
m/z


22-Nov-2013
15:08:36
TOF MS ES+
35.2
haoli1_167 iodo_Sar-1 14 (0.490) Sm (Mn, 2x3.00); Cm (9:19)
MS (ESI) of peptide **1b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[3M+4H]^{4+}$: *m/z* 1403.45
$[3M+3H+K]^{4+}$: *m/z* 1412.93
1404.1820
1403.9240
1404.4500
1403.6958
1404.6683
1413.6558
1413.4167
1413.9246
1404.9066
1414.1338
1413.1777
1405.0853
1414.4126
1403.4279
1414.6318
1399.9078
1409.1387
1409.9539
1418.9183
1419.9362
1423.1515
1400.1952
1408.9001
1410.1528
1418.6591
1423.8910
1401.1566
1415.9170
1427.9314
1394.4828
1397.8474
%
m/z

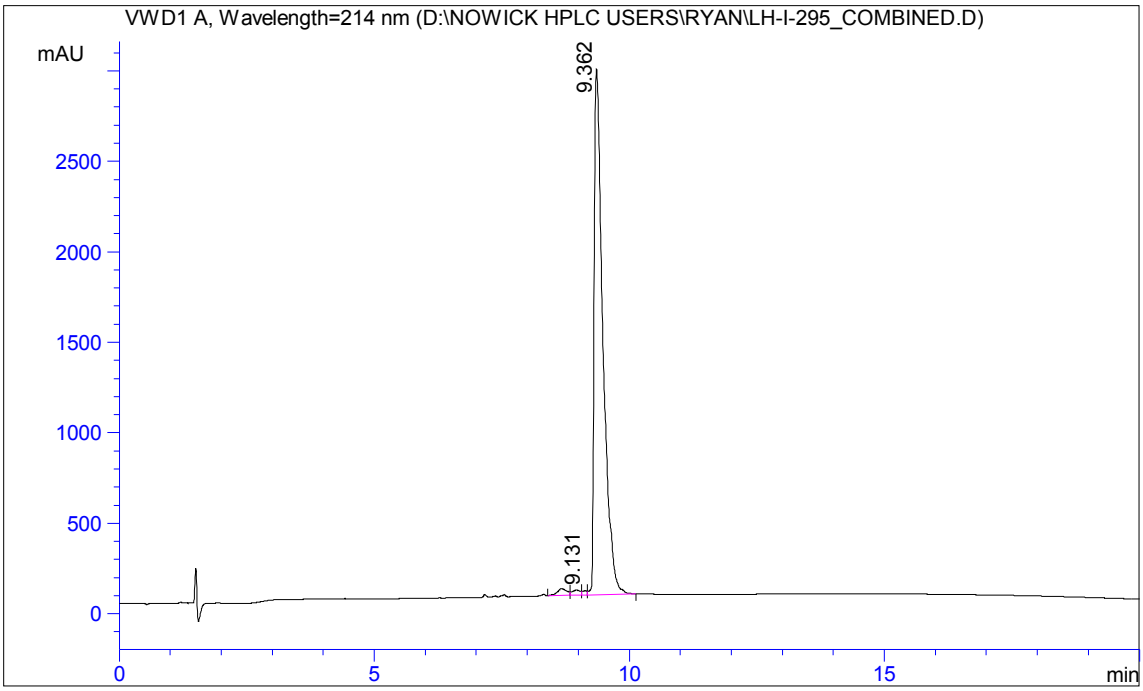


MS (ESI) of peptide **1b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+2H]^{2+}$: *m/z* 935.97
$[M+H+Na]^{2+}$: *m/z* 946.96



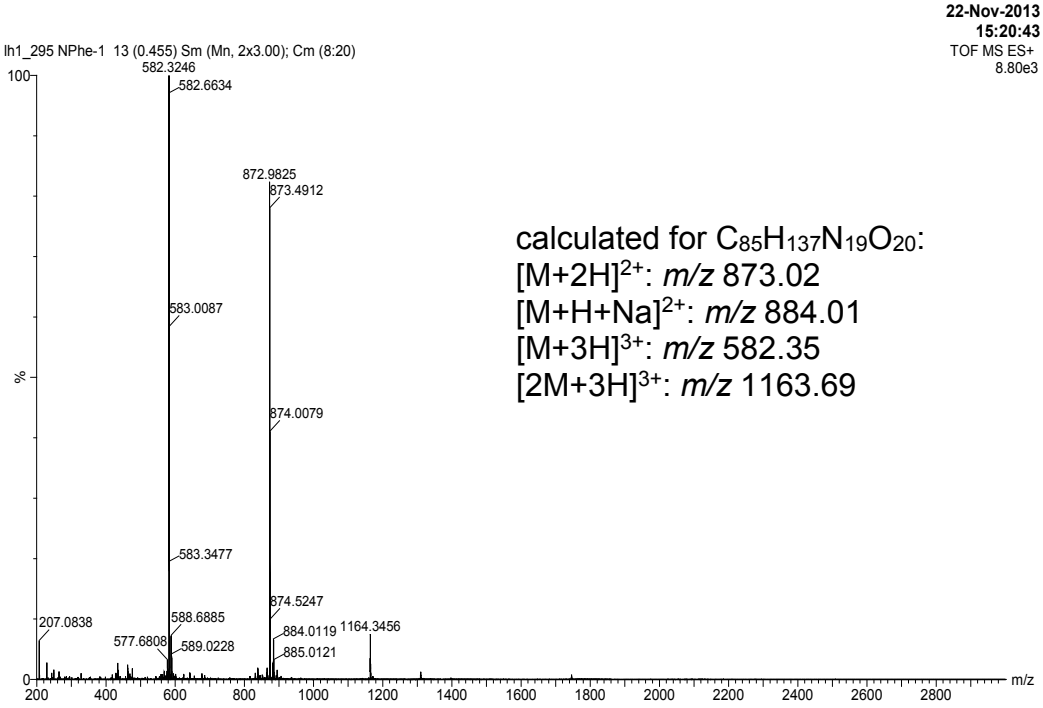
MS (ESI) of peptide **1b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+3H]^{3+}$: *m/z* 624.31
$[M+2H+Na]^{3+}$: *m/z* 631.64

HPLC and MS ESI+ TOF of peptide **2a**

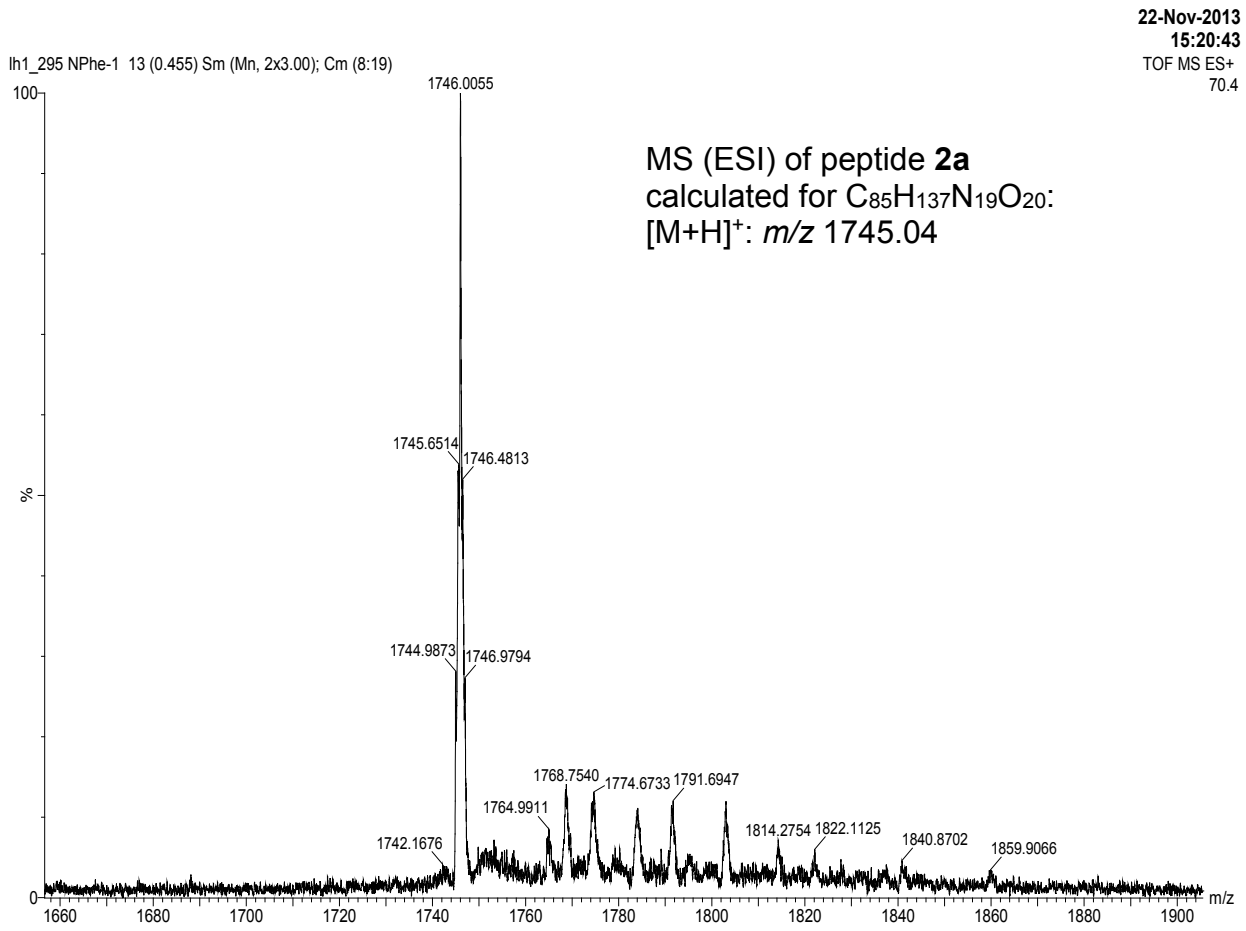


Signal 1:VWD1 A, Wavelength=214 nm

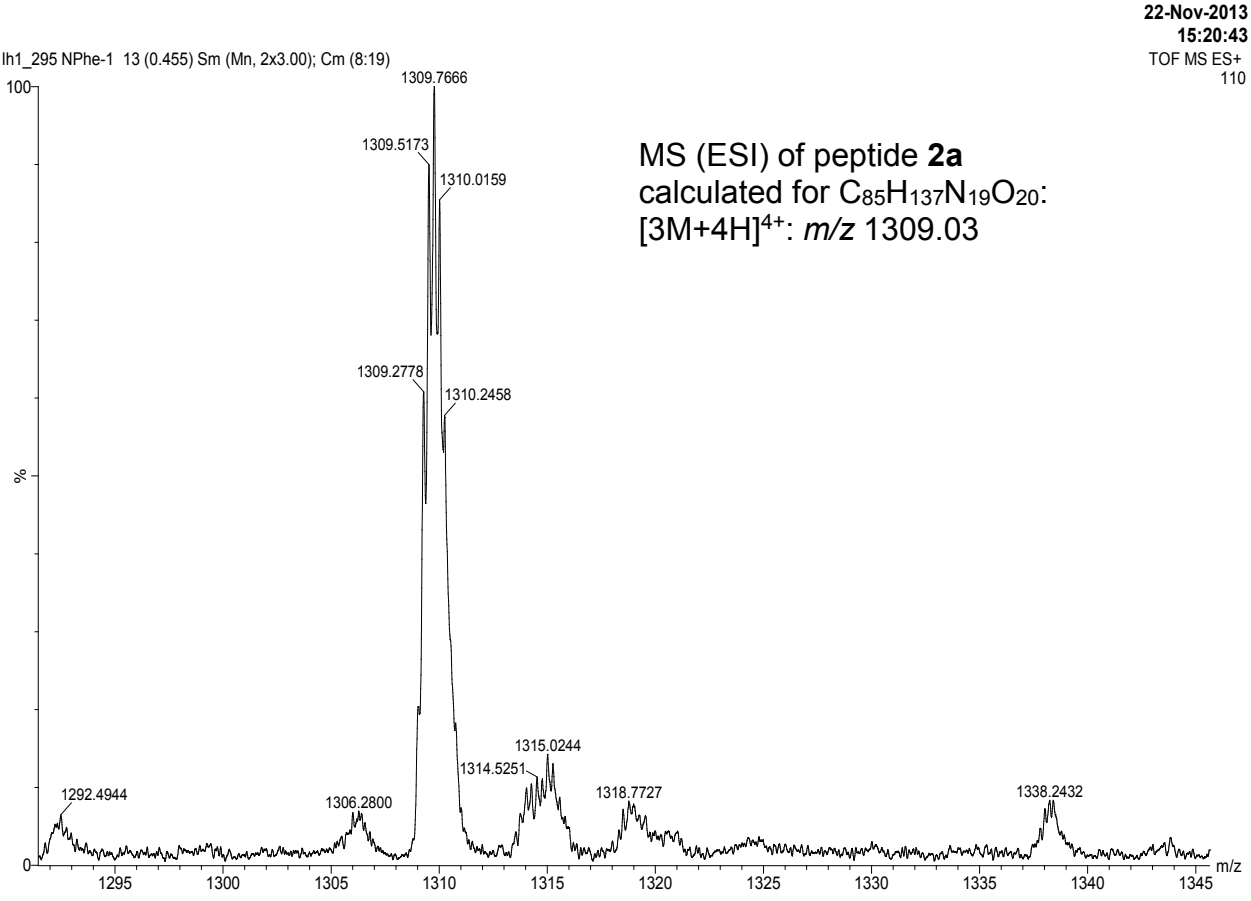
Peak #	RT [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	8.673	BV	0.189	516.040	1.280	1.440
2	8.966	VV	0.148	310.217	0.965	0.865
3	9.131	VV	0.091	146.465	0.773	0.409
4	9.362	VB	0.178	34871.512	96.982	97.286



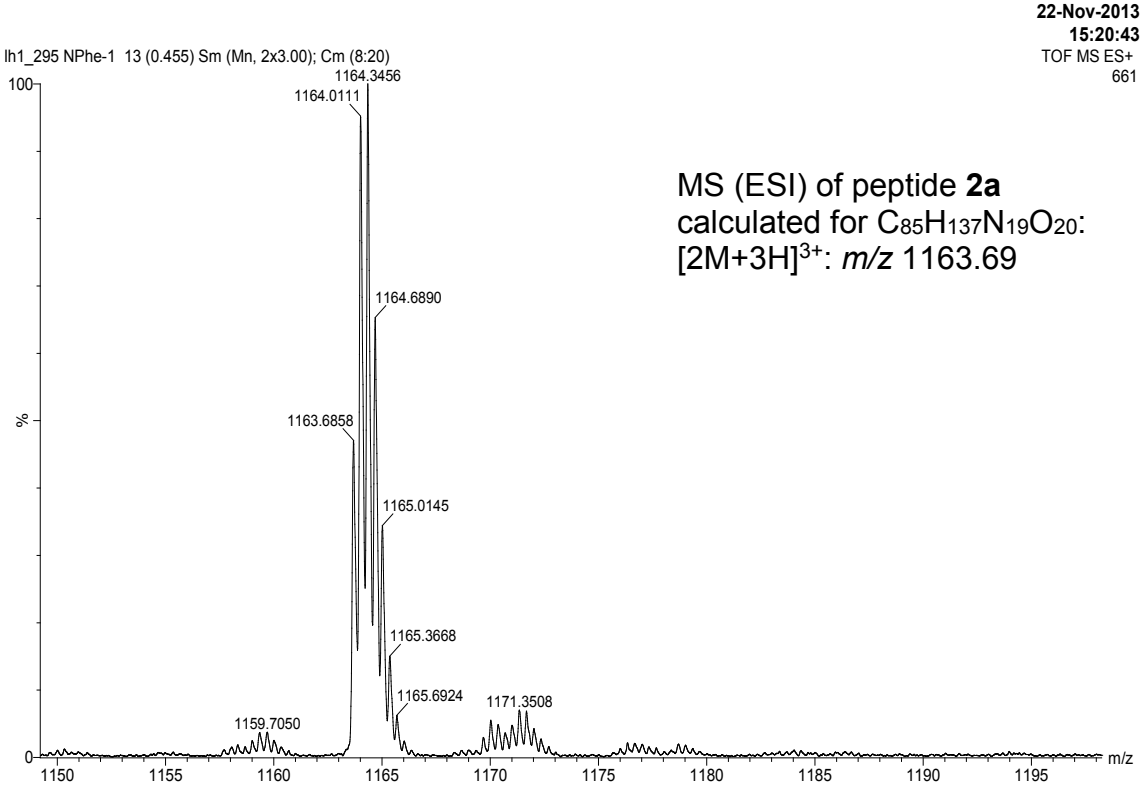
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+2H]^{2+}$: *m/z* 873.02
$[M+H+Na]^{2+}$: *m/z* 884.01
$[M+3H]^{3+}$: *m/z* 582.35
$[2M+3H]^{3+}$: *m/z* 1163.69



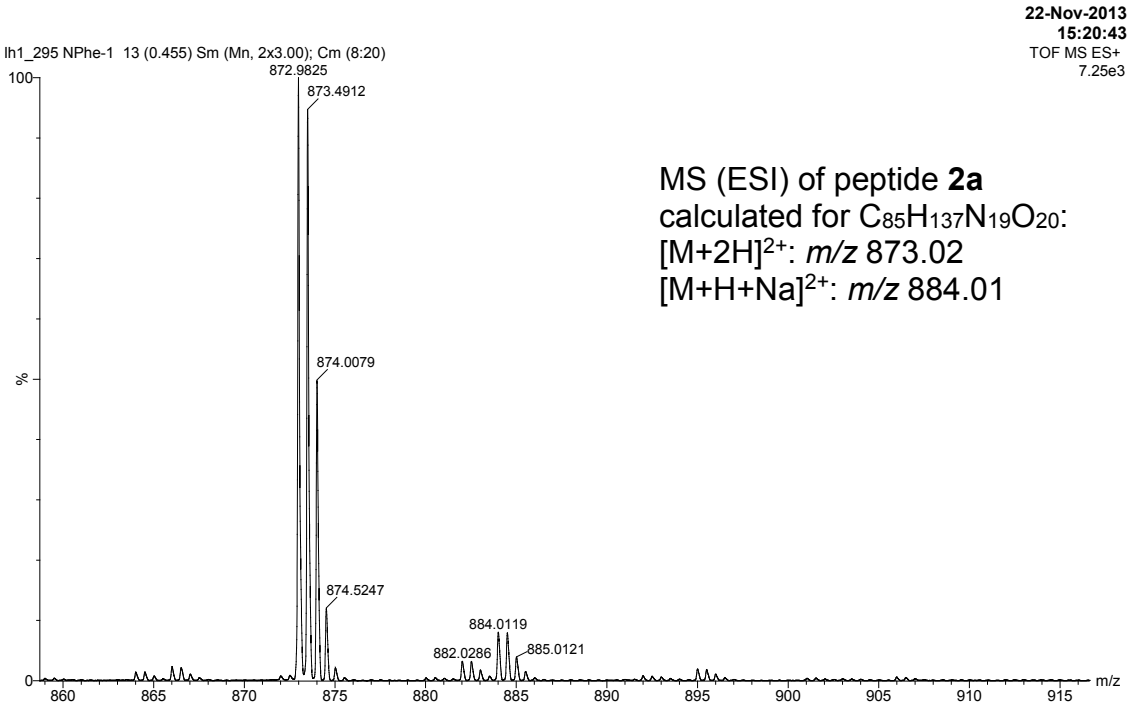
MS (ESI) of peptide **2a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+H]^+$: *m/z* 1745.04



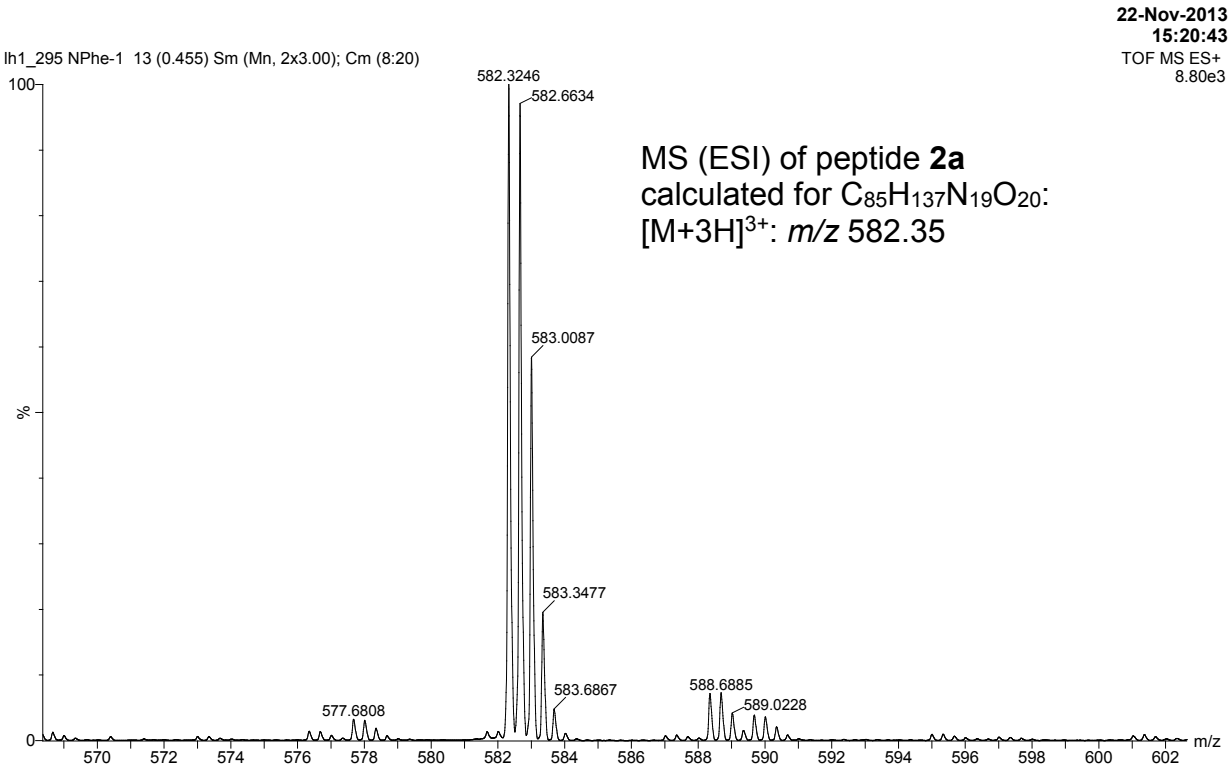
MS (ESI) of peptide **2a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[3M+4H]^{4+}$: *m/z* 1309.03



MS (ESI) of peptide **2a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[2M+3H]^{3+}$: *m/z* 1163.69

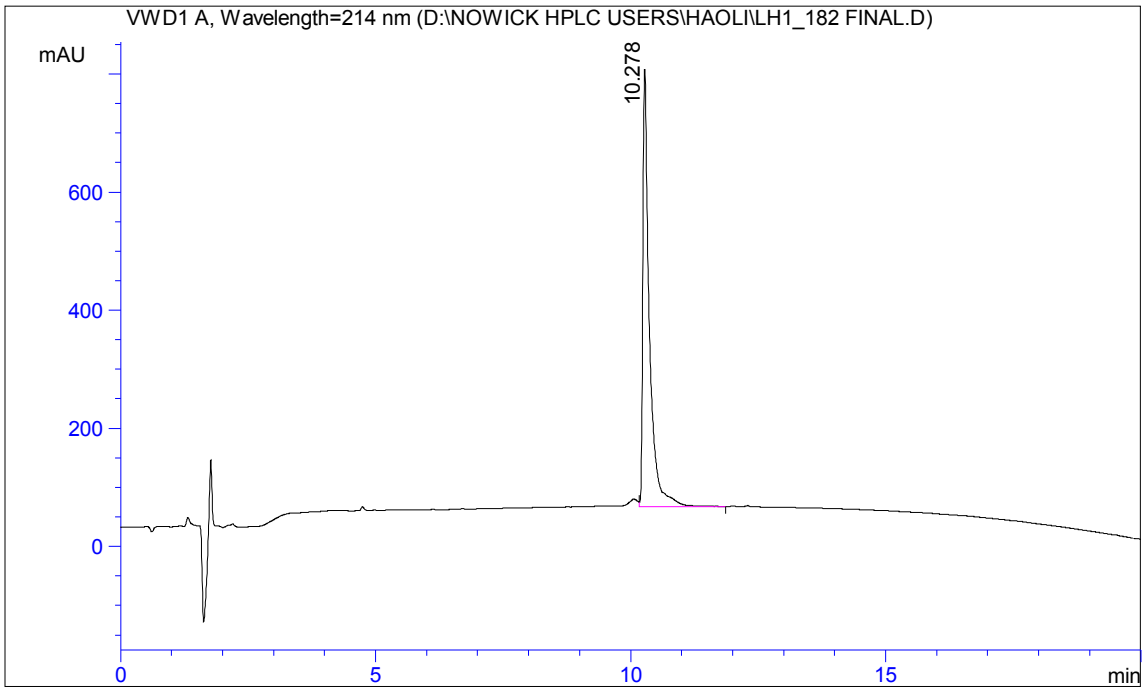


MS (ESI) of peptide **2a**
calculated for $C_{85}H_{137}N_{19}O_{20}$:
$[M+2H]^{2+}$: *m/z* 873.02
$[M+H+Na]^{2+}$: *m/z* 884.01



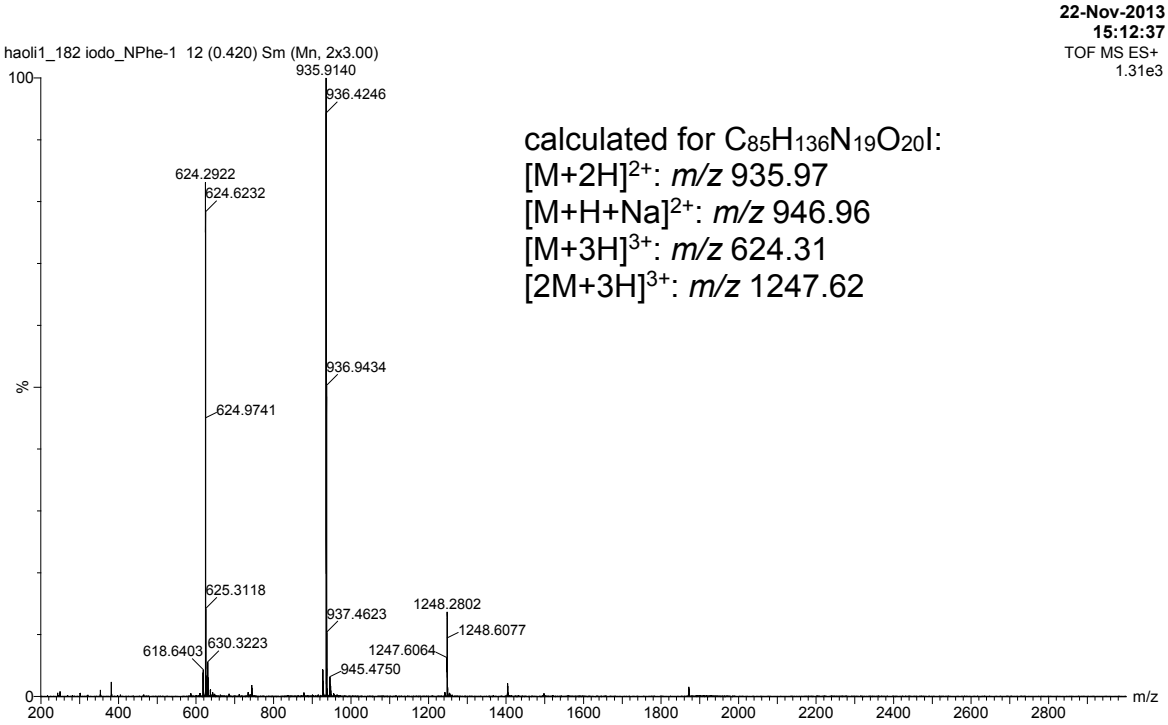
MS (ESI) of peptide **2a** calculated for $C_{85}H_{137}N_{19}O_{20}$: $[M+3H]^{3+}$: *m/z* 582.35

HPLC and MS ESI+ TOF of peptide **2b**

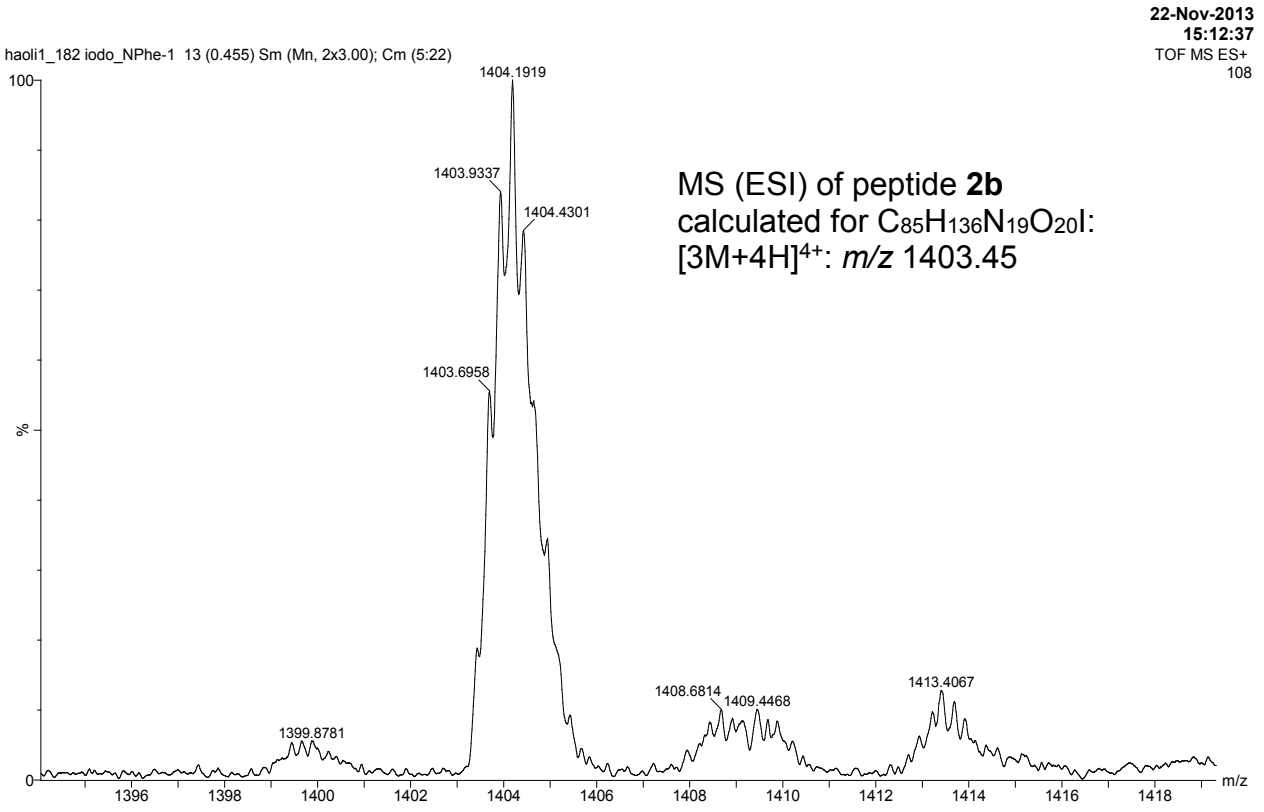


Signal 1:VWD1 A, Wavelength=214 nm

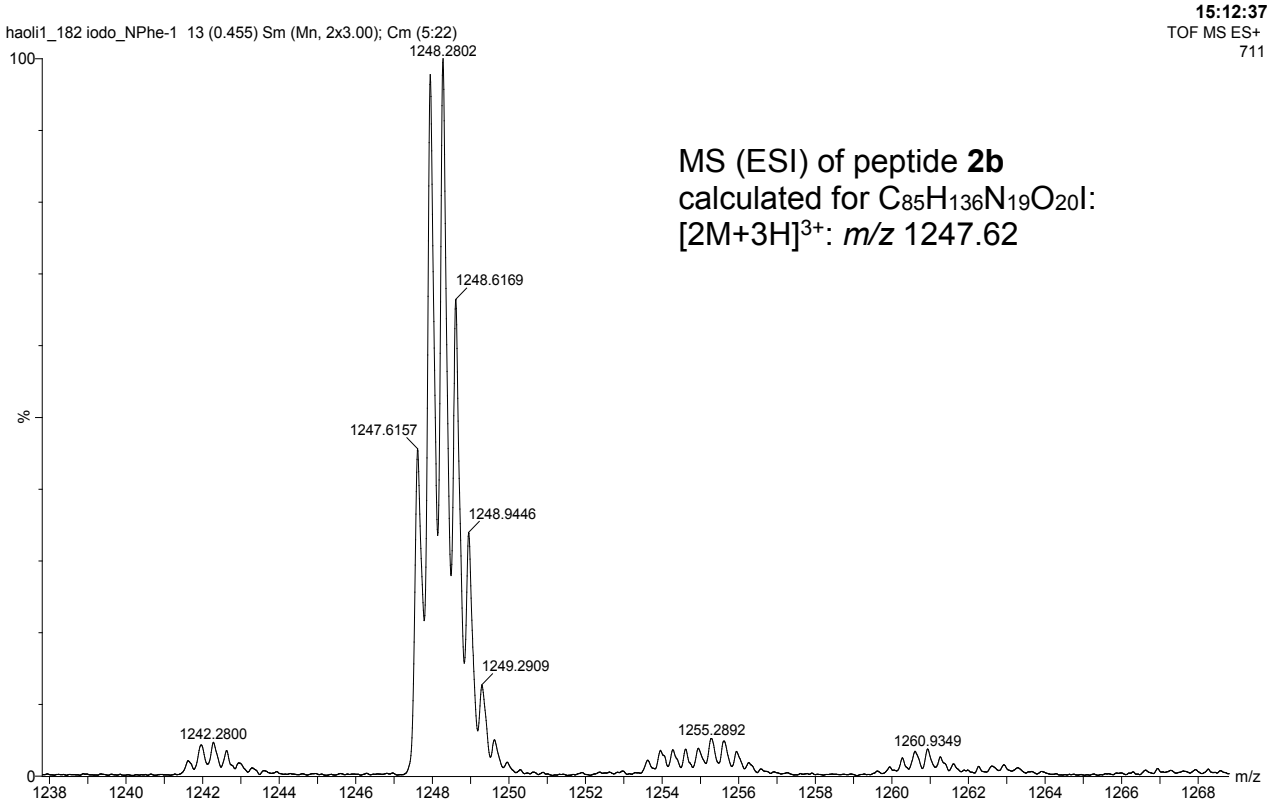
Peak #	RT [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	10.278	VV	0.128	6660.014	100.000	100.000



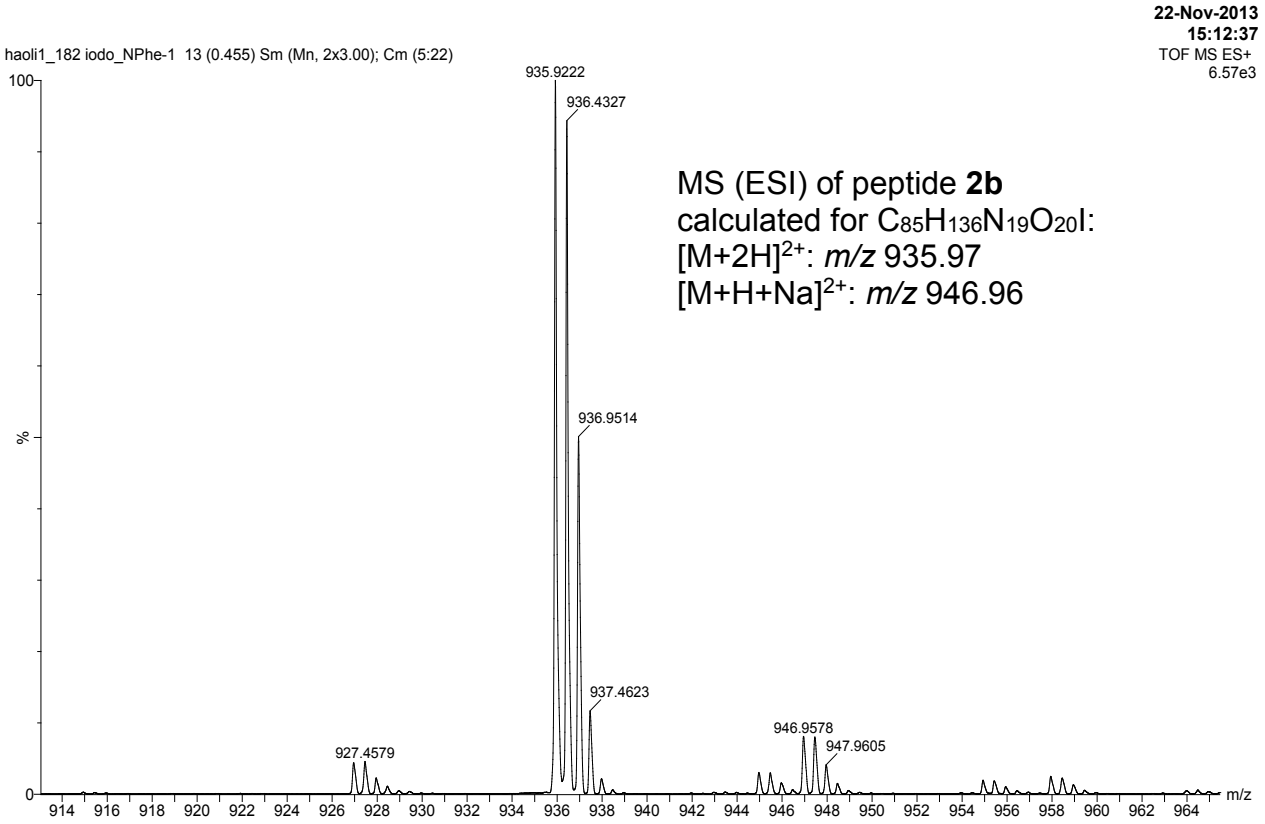
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+2H]^{2+}$: *m/z* 935.97
$[M+H+Na]^{2+}$: *m/z* 946.96
$[M+3H]^{3+}$: *m/z* 624.31
$[2M+3H]^{3+}$: *m/z* 1247.62

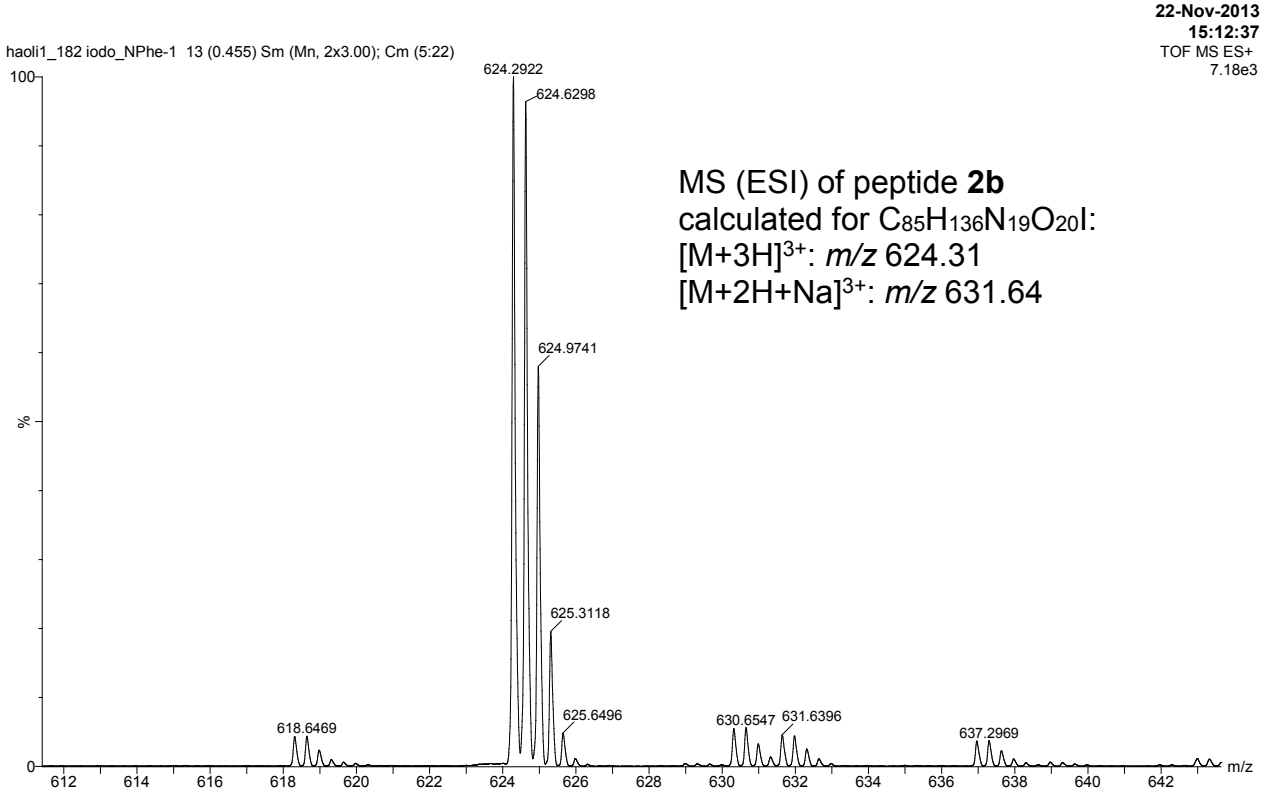


MS (ESI) of peptide **2b** calculated for $C_{85}H_{136}N_{19}O_{20}I$: $[3M+4H]^{4+}$: *m/z* 1403.45



MS (ESI) of peptide **2b** calculated for $C_{85}H_{136}N_{19}O_{20}I$: $[2M+3H]^{3+}$: *m/z* 1247.62


22-Nov-2013
15:12:37
TOF MS ES+
6.57e3
haoli1_182 iodo_NPhe-1 13 (0.455) Sm (Mn, 2x3.00); Cm (5:22)
935.9222
936.4327
936.9514
937.4623
927.4579
946.9578
947.9605
MS (ESI) of peptide **2b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+2H]^{2+}$: *m/z* 935.97
$[M+H+Na]^{2+}$: *m/z* 946.96
%
m/z


22-Nov-2013
15:12:37
TOF MS ES+
7.18e3
haoli1_182 iodo_NPhe-1 13 (0.455) Sm (Mn, 2x3.00); Cm (5:22)
624.2922
624.6298
624.9741
625.3118
625.6496
618.6469
630.6547
631.6396
637.2969
MS (ESI) of peptide **2b**
calculated for $C_{85}H_{136}N_{19}O_{20}I$:
$[M+3H]^{3+}$: *m/z* 624.31
$[M+2H+Na]^{3+}$: *m/z* 631.64
%
m/z