Electronic Supplementary Information

Controlling Amyloid Beta (Aβ) Peptide Aggregation and Toxicity by Protease Stable Ligands

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Table of Contents

1. Figure

1.1. Figure S1. Cellular viability of NT peptides by MTT assay.

1.2. Figure S2. Cellular viability in PC-12 derived neurons after treatment with Aβ42 peptide alone and Aβ42 peptide with NT peptides.

1.3. Figure S3. Cellular viability in PC-12-derived neurons after treatment with Aβ42 aggregates alone and Aβ42 aggregates with NT peptides.

1.4. Figure S4. Effects of NT peptides on Aβ42 aggregation measured by ThT assay.

1.5. Figure S5. BBB crossing of NT peptides, analysis by mass spectrometry.

1.6. Figure S6. Microscopic images of PC12 derived neurons.

2. Appendixes: HPLC and MALDI mass

2.1. Figure S7. HPLC chromatograph of NT-01.

2.2. Figure S8. HPLC chromatograph of NT-02.

2.3. Figure S9. HPLC chromatograph of NT-03.

2.4. Figure S10. HPLC chromatograph of NT-04.

2.5. Figure S11. HPLC chromatograph of NT-05.

2.6. Figure S12. HPLC chromatograph of NT-06.

2.7. Figure S13. HPLC chromatograph of NT-07.

2.8. Figure S14. HPLC chromatograph of NT-08.

2.9. Figure S15. HPLC chromatograph of NT-09.

2.10. Figure S16. HPLC chromatograph of NT-10.

2.11. Figure S17. HPLC chromatograph of NT-11.

2.12. Figure S18. HPLC chromatograph of NT-12.

2.13. Figure S19. HPLC chromatograph of NT-13.

2.14. Figure S20. HPLC chromatograph of NT-14.

2.15. Figure S21. HPLC chromatograph of KLVFF.

2.16. Figure S22. MALDI mass spectrum of NT-01.

2.17. Figure S23. MALDI mass spectrum of NT-02.

2.18. Figure S24. MALDI mass spectrum of NT-03.

2.19. Figure S25. MALDI mass spectrum of NT-04.

2.20. Figure S26. MALDI mass spectrum of NT-05.

2.21. Figure S27. MALDI mass spectrum of NT-06.

2.22. Figure S28. MALDI mass spectrum of NT-07.

2.23. Figure S29. MALDI mass spectrum of NT-08.

2.24. Figure S30. MALDI mass spectrum of NT-09.

2.25. Figure S31. MALDI mass spectrum of NT-10.

2.26. Figure S32. MALDI mass spectrum of NT-11.

2.27. Figure S33. MALDI mass spectrum of NT-12.

2.28. Figure S34. MALDI mass spectrum of NT-13.

2.29. Figure S35. MALDI mass spectrum of NT-14.

2.30. Figure S36. MALDI mass spectrum of KLVFF.

2.31. Figure S37. MALDI mass spectrum of FITC attached NT-02.

2.32. Figure S38. MALDI mass spectrum of FITC attached NT-03.

2.33. Figure S39. MALDI mass spectrum of FITC attached NT-13.

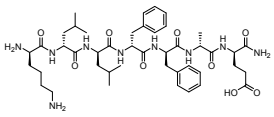
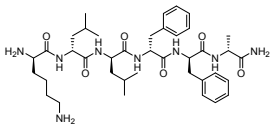
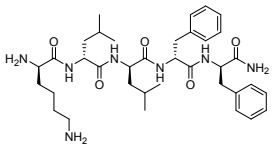
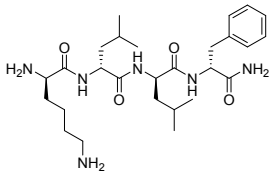
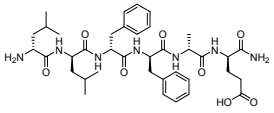
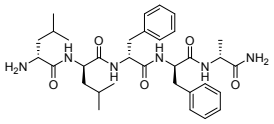
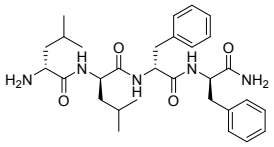
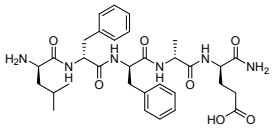
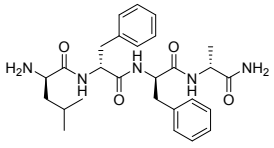
2.34. Figure S40. HRMS mass spectrum of NT-02.

2.35. Figure S41. HRMS mass spectrum of NT-03.

2.36. Figure S42. HRMS mass spectrum of NT-13.

2.37. Figure S43. HRMS mass spectrum of KLVFF.

Table S1. *Characterization and HPLC data of synthesized peptides*.

No.	Peptide sequence	Molecular formula	MASS		HPLC	
			Calculated	Obtained (M+H)	t_R (min)	Purity (%)
1		$C_{44}H_{67}N_9O_9$	865.5062	865.6390	5.196	100
2		$C_{39}H_{60}N_8O_6$	736.4636	737.7675	5.275	100
3		$C_{36}H_{55}N_7O_5$	665.4265	666.7092	5.298	100
4		$C_{27}H_{46}N_6O_4$	518.3581	519.3088	5.303	100
5		$C_{38}H_{55}N_7O_8$	737.4112	738.5652	5.301	100
6		$C_{33}H_{48}N_6O_5$	608.3686	609.4024	5.280	100
7		$C_{30}H_{43}N_5O_4$	537.3315	538.5833	5.232	100
8		$C_{32}H_{44}N_6O_7$	624.3271	625.3097	5.247	99.12
9		$C_{27}H_{37}N_5O_4$	495.2846	496.2403	5.156	100

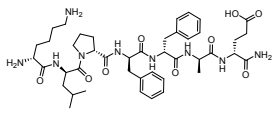
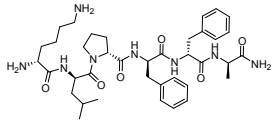
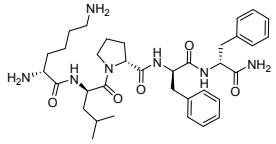
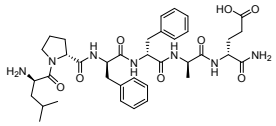
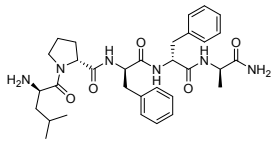
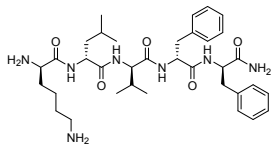
10		$C_{43}H_{63}N_9O_9$	849.4749	850.7135	5.201	100
11		$C_{38}H_{56}N_8O_6$	720.4323	720.6613	5.190	98.93
12		$C_{35}H_{51}N_7O_5$	649.3952	650.2834	5.251	100
13		$C_{37}H_{51}N_7O_8$	721.3799	721.1677	5.203	100
14		$C_{32}H_{44}N_6O_5$	592.3373	593.5271	5.178	99.58
15		$C_{35}H_{53}N_7O_5$	651.4108	652.3820	5.222	98.98
16	Aβ_{42}	NH_2- ^{1}DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGG VVIA^{42}-COOH				

Table S 2. *Cell viability of NT peptides in PC-12 derived neurons.*

S. No.	Peptide sequence	% Cell viability					
		Peptides concentration range (μM)					
		5	10	20	40	80	160
1	H_2N-KLLFFAE-NH_2	100.05	100.01	100.02	99.56	98.99	98.04
2	H_2N-KLLFFA-NH_2	99.79	98.72	97.25	95.57	92.14	91.01
3	H_2N-KLLFF-NH_2	100.03	99.85	99.05	99.56	98.99	98.95
4	H_2N-KLLF-NH_2	100	99.95	98.71	98.57	96.52	92.19
5	H_2N-LLFFAE-NH_2	100.02	99.91	98.26	97.23	95.62	91.28
6	H_2N-LLFFA-NH_2	98.85	92.54	86.00	80.87	75.78	71.68
7	H_2N-LLFF-NH_2	65.35	60.98	57.38	52.98	46.87	42.54
8	H_2N-LFFAE-NH_2	88.98	81.56	75.61	65.26	56.83	50.07
9	H_2N-LFFA-NH_2	100.05	98.01	96.53	90.24	85.62	78.29
10	H_2N-KLPFFAE-NH_2	100	98.12	95.98	91.47	85.12	79.31
11	H_2N-KLPFFA-NH_2	100	99.10	97.05	95.84	91.80	89.24
12	H_2N-KLPFF-NH_2	100	100.05	100	100	99.98	99.96
13	H_2N-LPFFAE-NH_2	100	99.52	99.01	97.34	95.71	91.67
14	H_2N-LPFFA-NH_2	100	100	100	100	99.91	99.50
15	H_2N-KLVFF-NH_2	100	100	100	100	100	100
16	Control	100					

*Each experiment was done in triplicates (n= 3). ODs (absorbance) of samples with untreated cells were set to 100. Taking the cell viability of untreated cells as 100, percentage cell viabilities were calculated for the samples treated with Aβ42 alone or plus the NT peptides. Subsequently, the percentage inhibition of Aβ toxicity by each test peptide was calculated by using the formula: Cell viability (%) = {[A570 (treated cells) - A570 (blank)]/ [A570 (control cells) - A570 (blank)]} *100. Blank ODs were subtracted from each sample OD and the triplicate ODs were averaged. In a subset of triplicate wells, OD readings did not deviate much from the mean and SD ranged between 1.12-6.4.

Table S 3. *Cell viability and neuroprotection effect of NT peptides against $A\beta_{42}$ induced toxicity in PC-12 derived neurons.*

S. No.	Peptide sequence	% Cell viability after treated with peptide and $A\beta_{42}$ (5 μM) peptide					
		Peptides concentration range (μM)					
		5	10	20	40	80	160
1	H_2N-KLLFFAE-NH_2	43.20	48.98	51.01	55.41	58.35	60.15
2	H_2N-KLLFFA-NH_2	75.13	79.69	80.72	85.87	86.08	90.18
3	H_2N-KLLFF-NH_2	76.64	76.73	75.30	82.14	85.81	88.24
4	H_2N-KLLF-NH_2	73.46	68.15	60.01	56.78	51.26	48.20
5	H_2N-LLFFAE-NH_2	74.38	69.91	66.34	61.12	58.84	56.42
6	H_2N-LLFFA-NH_2	62.61	58.25	54.21	48.07	42.19	38.24
7	H_2N-LLFF-NH_2	35.54	32.19	29.51	23.78	19.98	19.26
8	H_2N-LFFAE-NH_2	44.35	43.15	38.02	25.91	20.75	15.67
9	H_2N-LFFA-NH_2	40.33	41.05	45.08	47.50	49.35	48.32
10	H_2N-KLPFFAE-NH_2	50.19	55.06	56.53	58.73	60.24	62.63
11	H_2N-KLPFFA-NH_2	60.08	58.67	55.54	50.15	50.86	49.13
12	H_2N-KLPFF-NH_2	63.10	64.98	66.31	68.01	69.08	71.06
13	H_2N-LPFFAE-NH_2	76.08	84.16	82.27	84.62	83.02	85.58
14	H_2N-LPFFA-NH_2	60.58	63.24	64.15	66.20	67.68	67.52
15	H_2N-KLVFF-NH_2	72.08	73.60	77.06	80.36	83.13	83.79
16	Control	100					
17	$A\beta_{42}$	38.05					

*Each experiment was done in triplicates (n= 3). ODs (absorbance) of samples with untreated cells were set to 100. Taking the cell viability of untreated cells as 100, percentage cell viabilities were calculated for the samples treated with Aβ42 alone or plus the NT peptides. Subsequently, the percentage inhibition of Aβ toxicity by each test peptide was calculated by using the formula: Cell viability (%) = {[A570 (treated cells) - A570 (blank)]/ [A570 (control cells) - A570 (blank)]} *100. Blank ODs were subtracted from each sample OD and the triplicate ODs were averaged. In a subset of triplicate wells, OD readings did not deviate much from the mean and SD ranged between 1.09-6.2.

Table S 4. *Cell viability and neuroprotection effect of NT peptides against $A\beta_{42}$ induced toxicity in PC-12 derived neurons.*

S. No.	Peptide sequence	% Cell viability after treated with peptides and $A\beta_{42}$ (5 μM) aggregates					
		Peptides concentration range (μM)					
		5	10	20	40	80	160
1	H_2N-KLLFFAE-NH_2	62.30	64.19	65.60	68.49	72.57	75.27
2	H_2N-KLLFFA-NH_2	84.36	85.91	88.07	90.10	93.24	94.30
3	H_2N-KLLFF-NH_2	82.64	84.73	85.30	87.56	90.81	92.41
4	H_2N-KLLF-NH_2	76.24	78.08	80.20	81.58	82.36	84.23
5	H_2N-LLFFAE-NH_2	68.82	69.52	70.34	72.10	75.18	76.14
6	H_2N-LLFFA-NH_2	52.23	48.69	44.81	42.02	42.09	40.80
7	H_2N-LLFF-NH_2	55.15	53.21	50.83	44.61	39.12	31.75
8	H_2N-LFFAE-NH_2	53.08	50.06	48.69	42.09	38.38	35.16
9	H_2N-LFFA-NH_2	68.62	65.05	63.28	62.23	59.15	56.09
10	H_2N-KLPFFAE-NH_2	65.24	63.98	62.15	60.98	59.23	58.14
11	H_2N-KLPFFA-NH_2	72.35	65.98	60.17	57.06	56.15	55.54
12	H_2N-KLPFF-NH_2	73.10	75.57	76.96	77.41	81.22	83.06
13	H_2N-LPFFAE-NH_2	82.35	85.52	87.16	89.32	90.14	92.16
14	H_2N-LPFFA-NH_2	72.18	73.02	73.77	74.02	75.56	76.05
15	H_2N-KLVFF-NH_2	78.01	81.02	84.16	86.12	87.35	89.23
16	Control	100					
17	$A\beta_{42}$	43.27					

*Each experiment was done in triplicates (n=3). ODs (absorbance) of samples with untreated cells were set to 100. Taking the cell viability of untreated cells as 100, percentage cell viabilities were calculated for the samples treated with Aβ42 alone or plus the NT peptides. Subsequently, the percentage inhibition of Aβ toxicity by each test peptide was calculated by using the formula: Cell viability (%) = {[A570 (treated cells) - A570 (blank)]/ [A570 (control cells) - A570 (blank)]} *100. Blank ODs were subtracted from each sample OD and the triplicate ODs were averaged. In a subset of triplicate wells, OD readings did not deviate much from the mean and SD ranged between 1.9-6.7.

Table S5. *ThT assay and inhibition of $A\beta_{42}$ aggregation.*

Peptides	% Of $A\beta_{42}$ aggregations after treated with NT peptides					
	NT Peptides concentration range (μM)					
	5	**10**	**20**	**40**	**80**	**160**
NT-01	72.71	68.16	65.52	63.95	60.15	61.04
NT-02	42.39	36.33	29.77	25.57	22.14	21.04
NT-03	45.74	35.71	25.34	21.56	20.63	19.37
NT-04	52.86	50.57	49.80	48.52	45.67	40.10
NT-05	55.36	50.14	48.64	44.52	40.65	41.29
NT-06	56.64	53.41	53.63	51.36	43.14	40.64
NT-07	90.32	86.31	75.03	65.98	64.87	62.50
NT-08	56.17	54.47	52.57	50.10	48.44	45.70
NT-09	51.75	48.40	46.50	42.24	40.20	38.59
NT-10	72.44	66.96	54.04	47.48	45.25	43.14
NT-11	58.94	55.67	53.37	52.80	50.25	48.46
NT-12	60.38	57.62	55.24	52.10	20.21	50.10
NT-13	51.59	35.61	24.49	23.15	22.25	20.12
NT-14	75.15	70.80	68.02	51.78	45.82	41.05
NT-15	58.13	55.02	48.04	39.18	35.98	30.29
$A\beta_{42}$ Alone	100					

*Each experiment was done in triplicates (n= 3). ThT fluorescence intensity of samples Aβ42 alone was set to 100. Taking the aggregation Aβ42 alone as 100, % of aggregation was calculated for the samples Aβ42 treated with the NT peptides. Subsequently, the % aggregation of each peptide was calculated by using the formula: Aggregation (%) = {[Fl482 (treated cells)]/ [FI482 (Aβ42 alone control)]} *100. The triplicate fluorescence intensity (FI) was averaged. In a subset of triplicate test samples, FIs readings did not deviate much from the mean and SD ranged between 2.16-5.2.

Table S6. *Molecular docking studies of NT peptides with Aβ42 (PDB ID: 1Z0Q) and the binding modes with affinity.*

No. of modes	The binding affinity of NT-02 towards Aβ42 (kcal/mol)	The binding affinity of NT-03 towards Aβ42 (kcal/mol)	The binding affinity of NT-13 towards Aβ42 (kcal/mol)
1	-5.2	-5.3	-4.5
2	-5.1	-4.9	-4.3
3	-5.1	-4.7	-4.3
4	-5.1	-4.7	-4.3
5	-5.1	-4.7	-4.3
6	-5.1	-4.6	-4.2
7	-5.0	-4.6	-4.1
8	-5.0	-4.6	-4.1
9	-5.0	-4.5	-4.0
10	-4.9	-4.5	-4.0
11	-4.8	-4.4	-4.0
12	-4.8	-4.4	-3.9
13	-4.7	-4.4	-3.9
14	-4.7	-4.3	-3.9
15	-4.7	-4.3	-3.9
16	-4.6	-4.2	-3.9
17	-4.6	-4.2	-3.8
18	-4.6	-4.2	-3.8
19	-4.6	-4.2	-3.8
20	-4.6	-4.1	-3.7

Table S7. *Animal studies information. (Sex, source, species, number of animals, strains, route, dose*

Group	Sample	Sex	Age (weeks)	Weight (gram)	Dose (5mg/kg) 0.1 mL
1	Sucrose	Female	8-10	54.38	0.27 mg
		Female	8-10	53.71	0.26 mg
		Female	8-10	57.08	0.28 mg
2	NT-02	Female	8-10	58.68	0.29 mg
		Female	8-10	51.96	0.25 mg
		Female	8-10	59.55	0.29 mg
3	NT-03	Female	8-10	52.17	0.26 mg
		Female	8-10	53.67	0.26 mg
		Female	8-10	56.92	0.28 mg
4	NT-13	Female	8-10	56.66	0.26 mg
		Female	8-10	55.16	0.27 mg
		Female	8-10	54.63	0.27 mg
Source	CSIR-IICB, Kolkata				
Species	Mice				
Strain	C57BL/6J				
Route	Intra Peritoneal				

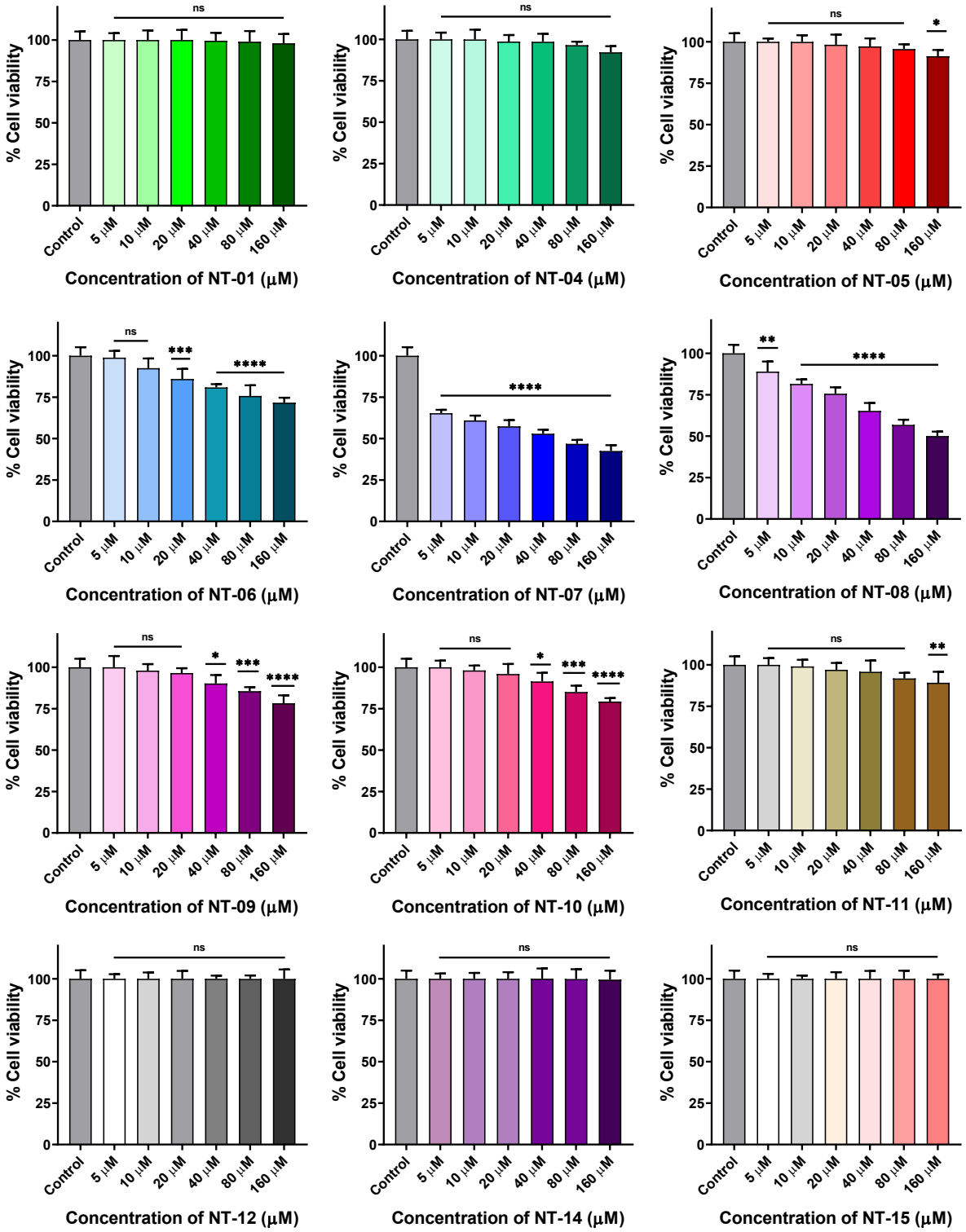


Figure S1. Cellular viability of NT peptides with various concentrations 5, 10, 20, 40, 80, and 160 μM in PC-12 derived neurons by using MTT assay.

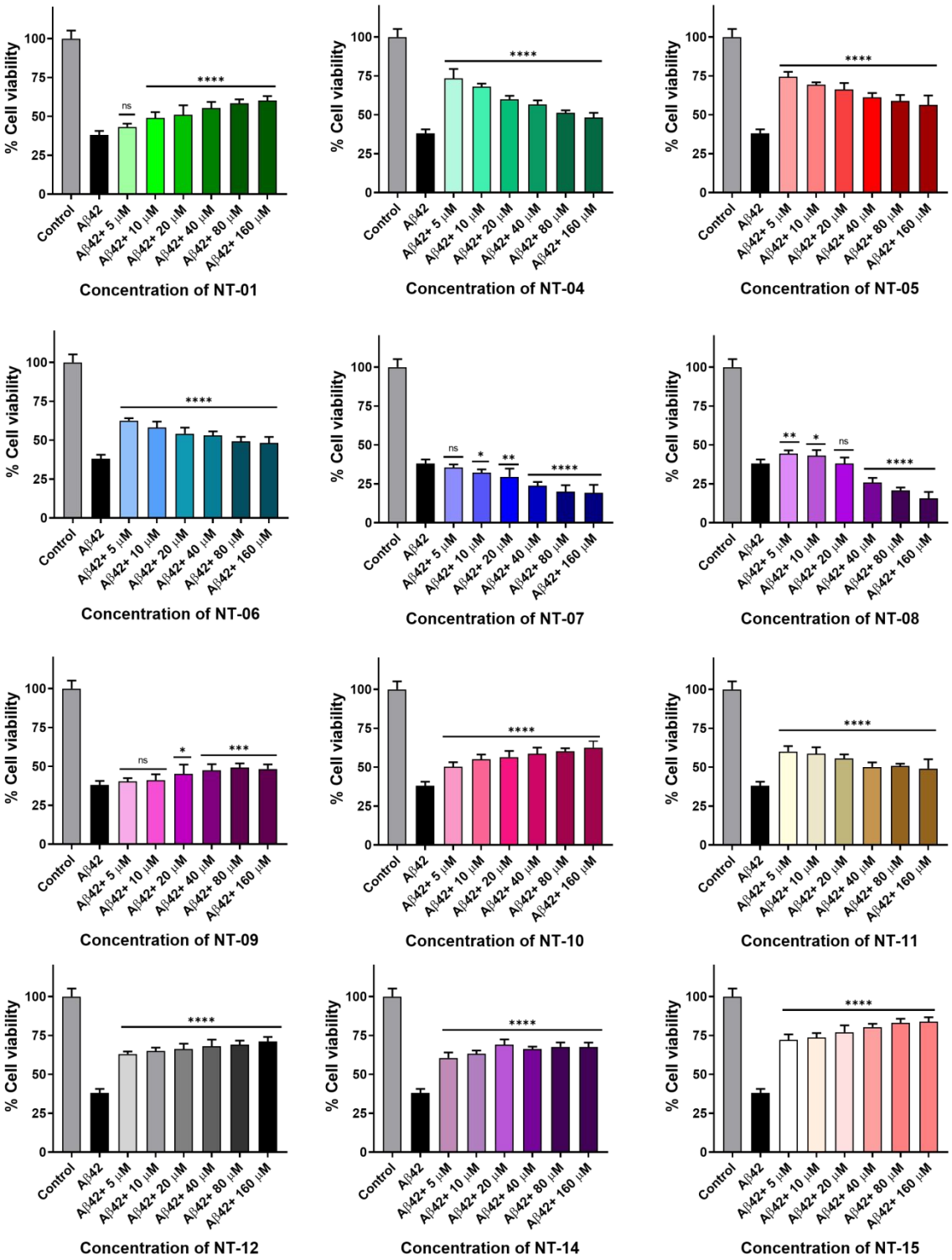


Figure S2. Cellular viability. After treatment with Aβ42 peptide alone and Aβ42 peptide with NT peptides with various concentrations 5, 10, 20, 40, 80, and 160 μM and in PC-12 derived neurons by using MTT assay.

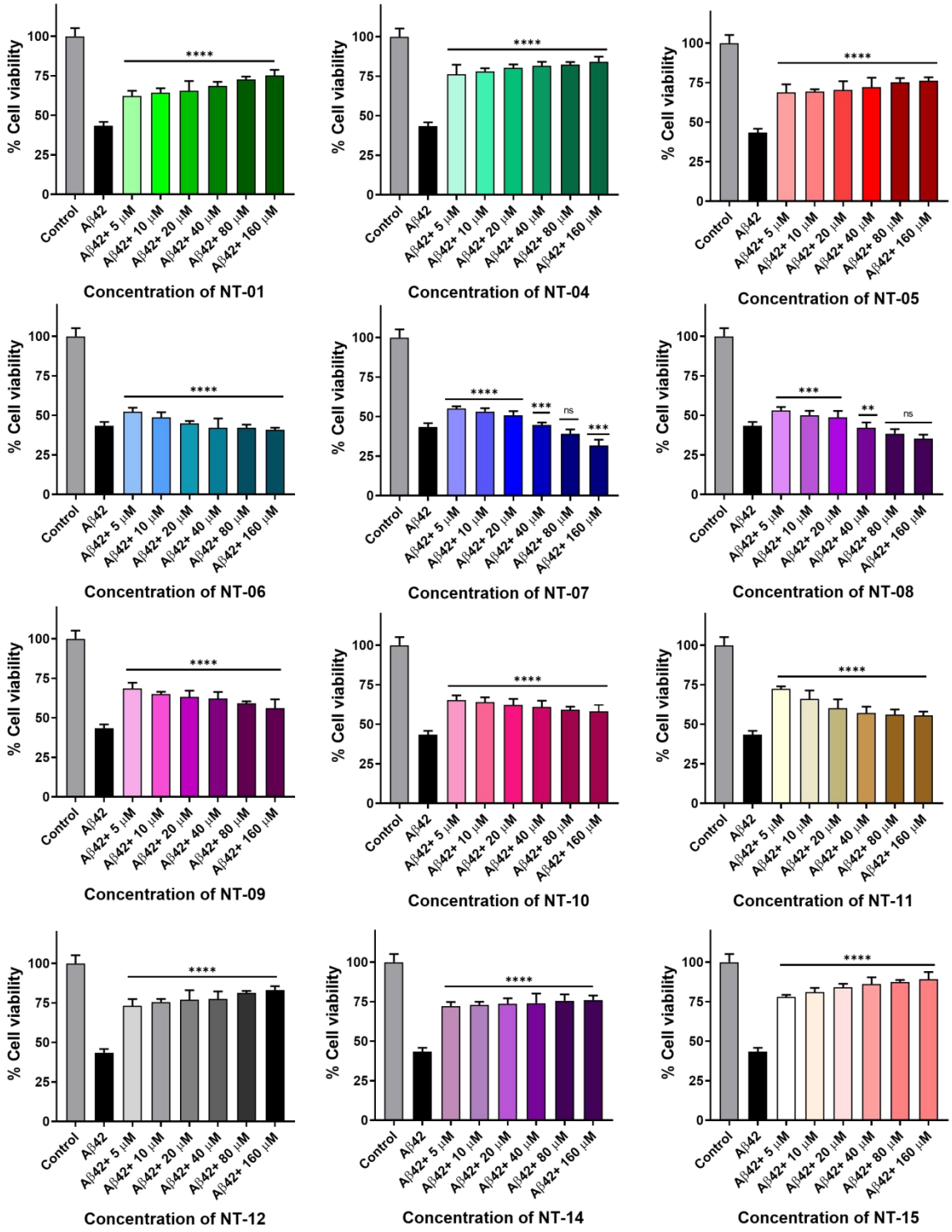


Figure S3. Cellular viability. After treatment with Aβ42 aggregates alone and Aβ42 aggregates with NT peptides with various concentrations 5, 10, 20, 40, 80, and 160 μM and in PC-12 derived neurons by using MTT assay.

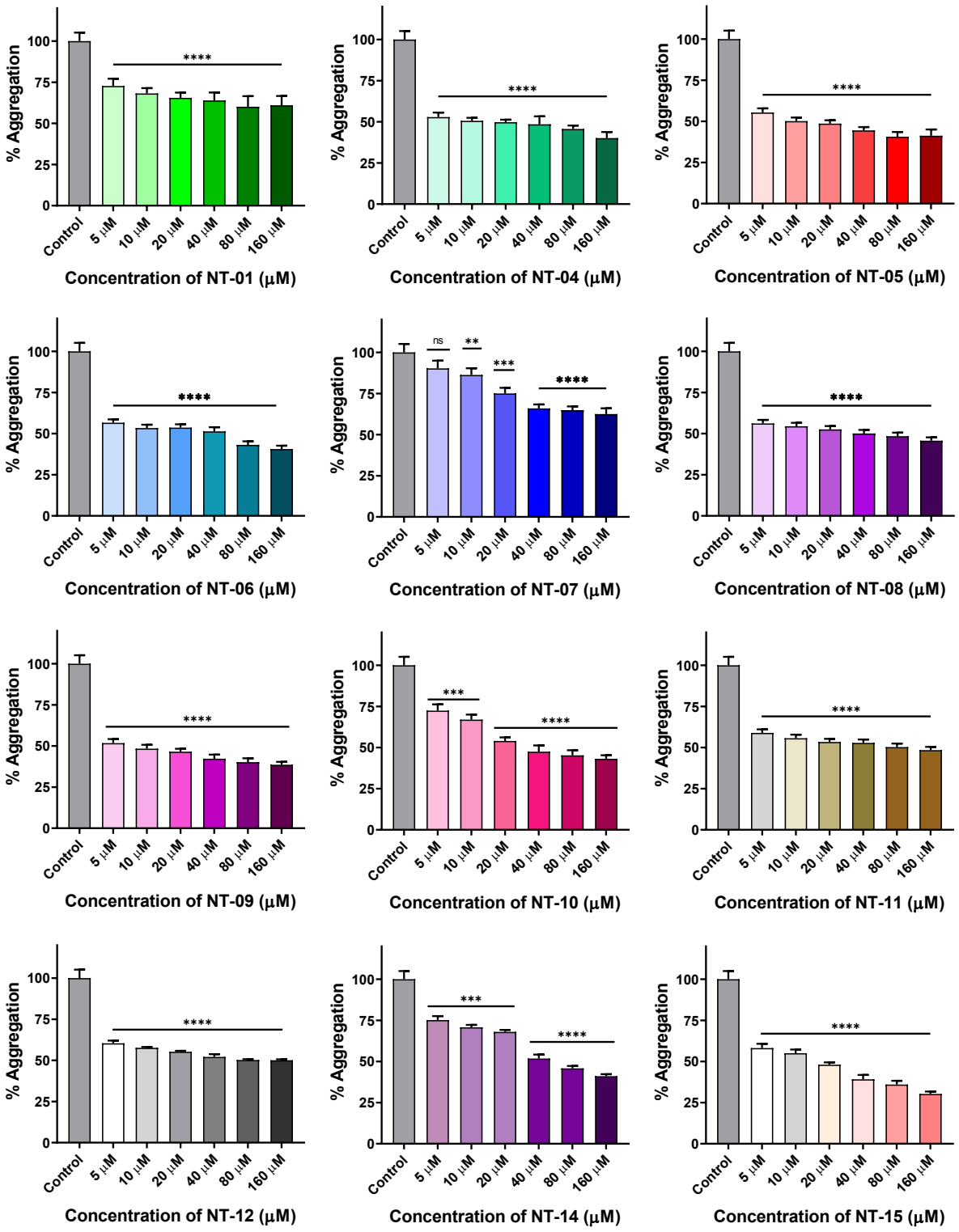


Figure S4. Effects of NT peptides on Aβ42 aggregation measured by ThT fluorescence intensity.

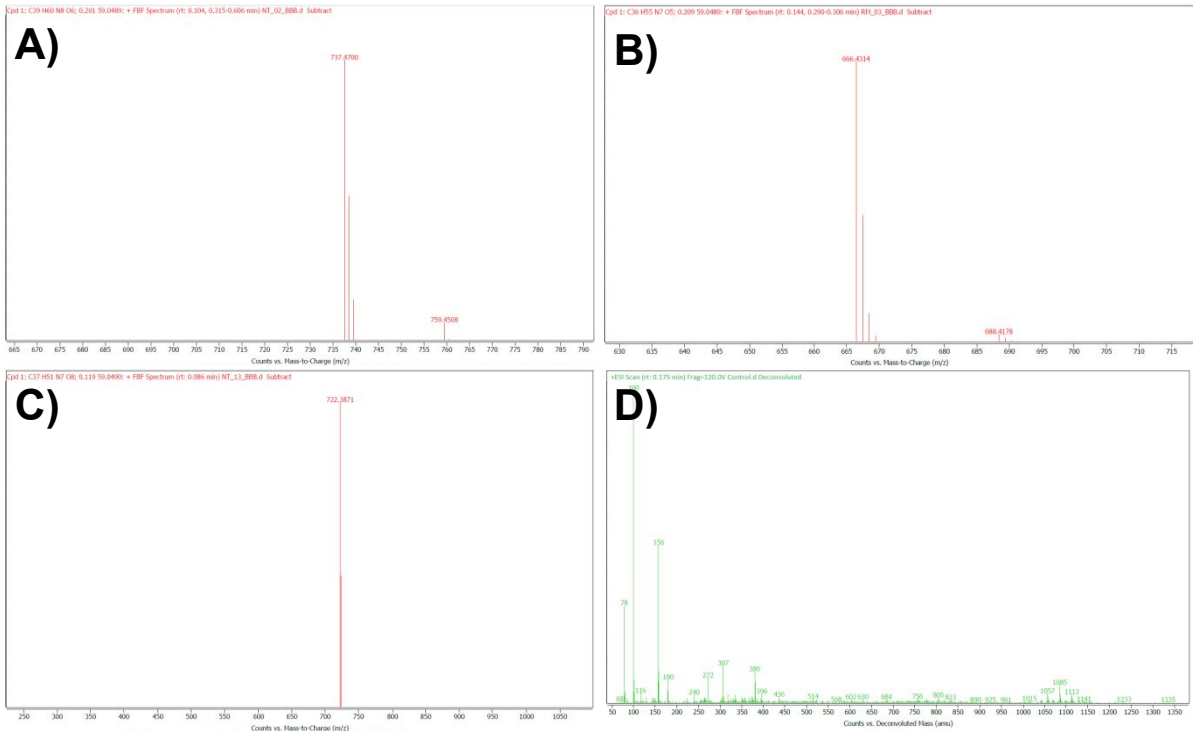


Figure S5. BBB crossing by NT peptides and analysed with HRMS mass spectrometry A) NT-02 peptide was identified by the major mass peak at M+H = 737.4700 B) NT-03 peptide was identified by the major mass peak at M+H =666.4314. C) NT-13 peptide was identified by the major mass peak at M+H = 722.3871. D) Control experiment of BBB crossing by sucrose and there is no mass peak at 342.2965.

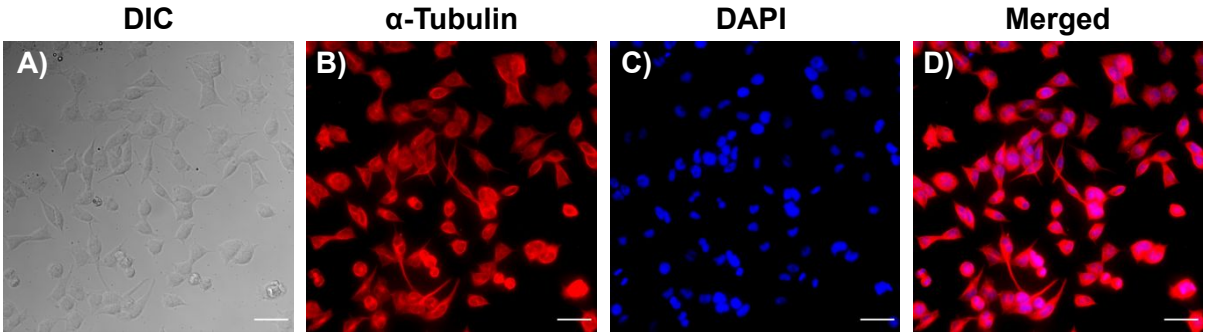
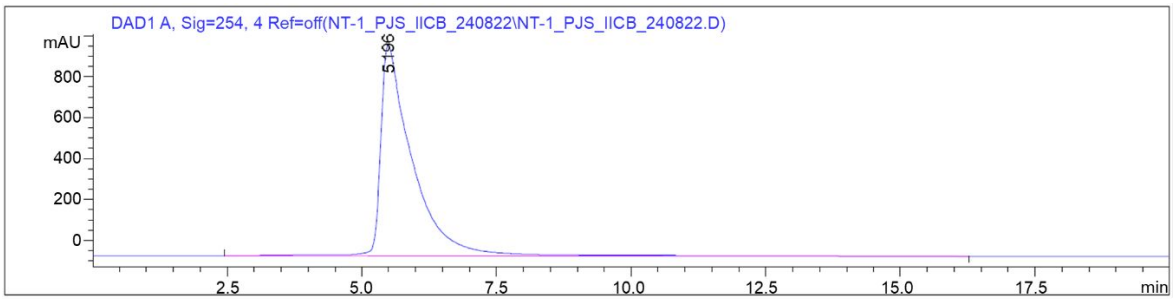


Figure S6. Microscopic images of PC12 derived neurons (a) DIC mode (b) TRITC channel (c) DAPI channel and (d) merged channel. Scale bar corresponding to 50 µm.

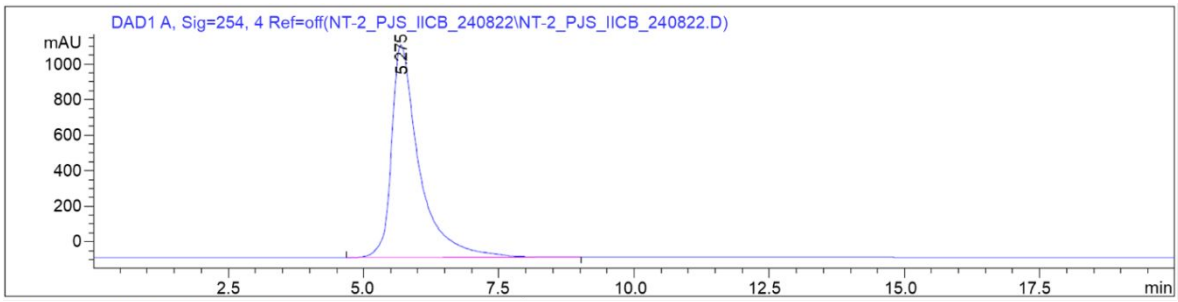
2. Appendixes: HPLC spectra and MALDI mass spectra.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.196	BB	0.2271	1.72764e4	1032.89001	100.0000
Totals :				1.72764e4	1032.89001	

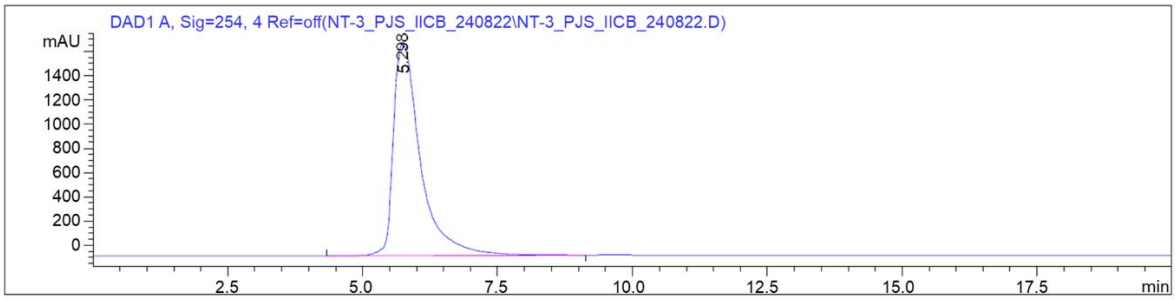
Figure S7. HPLC chromatogram of NT-01 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.275	BB	0.2065	1.70377e4	1194.11194	100.0000
Totals :				1.70377e4	1194.11194	

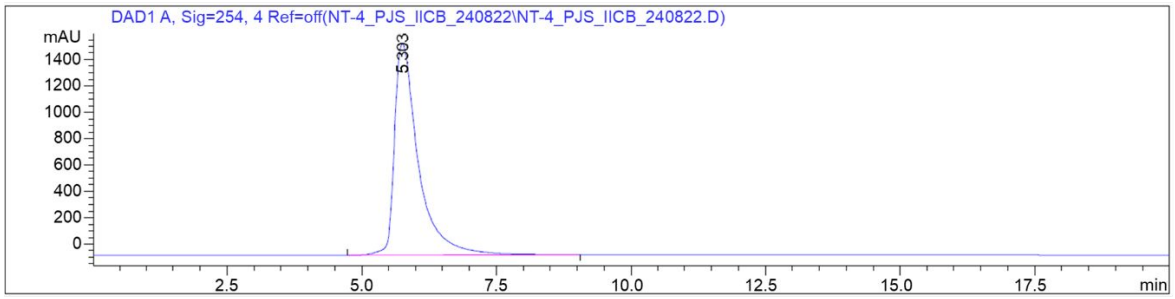
Figure S8. HPLC chromatogram of NT-02 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.298	BB	0.2131	2.44451e4	1748.11816	100.0000
Totals :				2.44451e4	1748.11816	

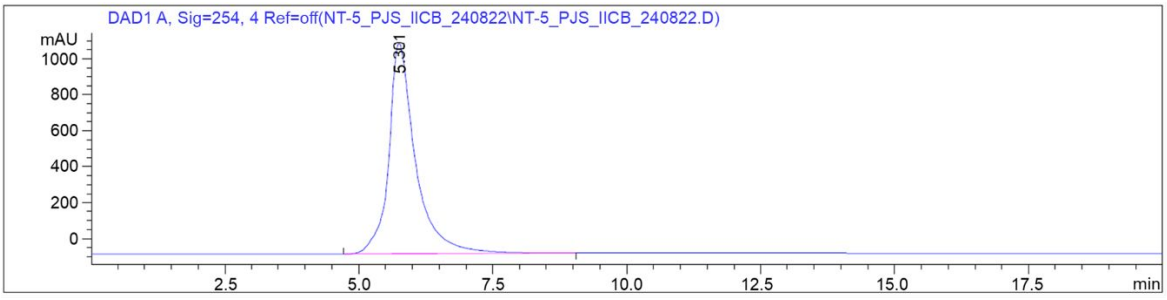
Figure S9. HPLC chromatogram of NT-03 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.303	BB	0.1826	1.98832e4	1603.70129	100.0000
Totals :				1.98832e4	1603.70129	

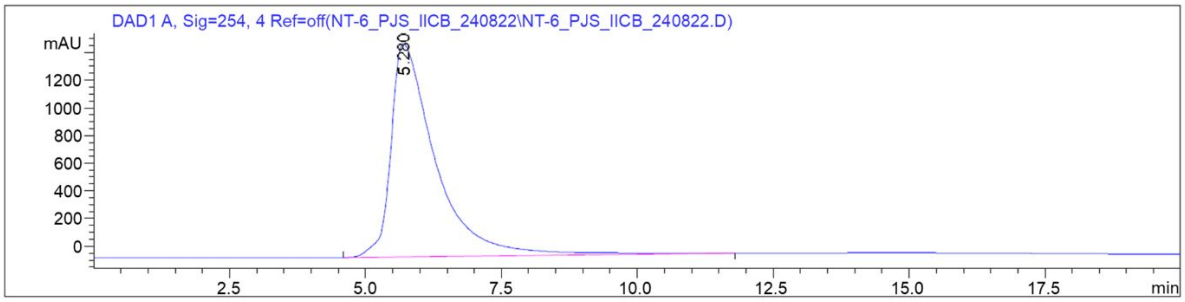
Figure S10. HPLC chromatogram of NT-04 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.301	BB	0.2006	1.63177e4	1170.81750	100.0000
Totals :				1.63177e4	1170.81750	

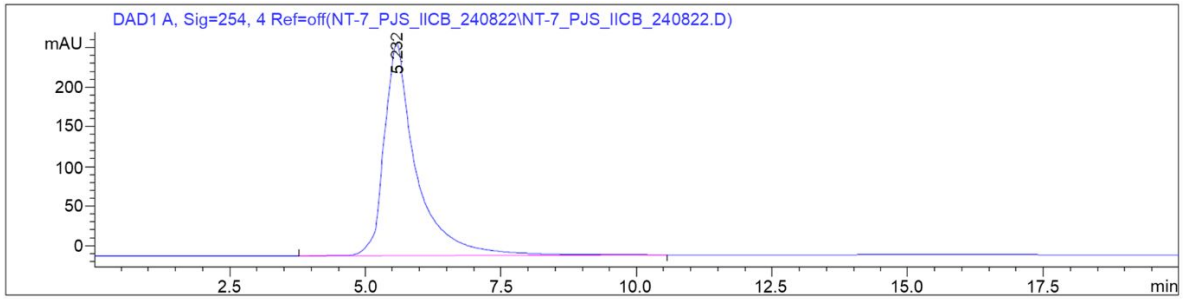
Figure S11. HPLC chromatogram of NT-05 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.280	BB	0.3350	3.54736e4	1538.69580	100.0000
Totals :				3.54736e4	1538.69580	

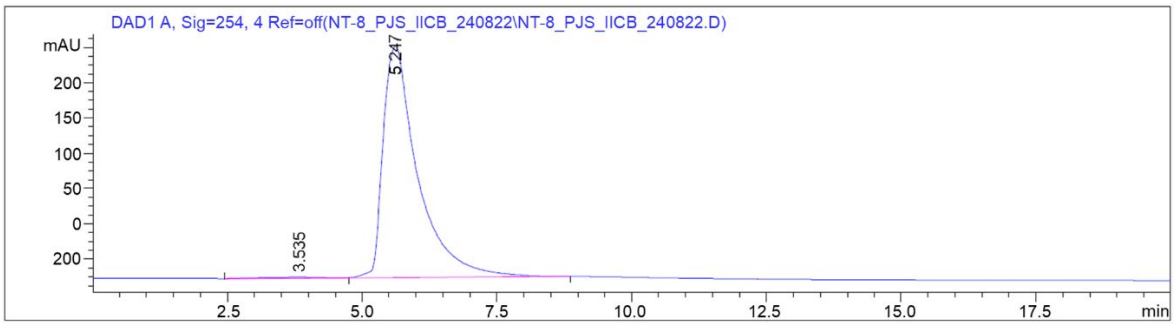
Figure S12. HPLC chromatogram of NT-06 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.232	BB	0.2231	4395.56006	268.37292	100.0000
Totals :				4395.56006	268.37292	

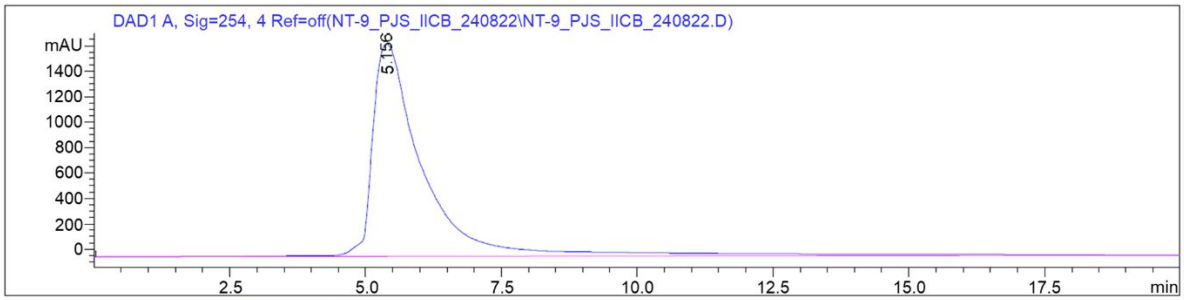
Figure S13. HPLC chromatogram of NT-07 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.535	BV E	0.4205	206.98911	6.44752	0.8702
2	5.247	VB R	0.2655	2.35679e4	1313.08923	99.1298
Totals :				2.37869e4	1319.53775	

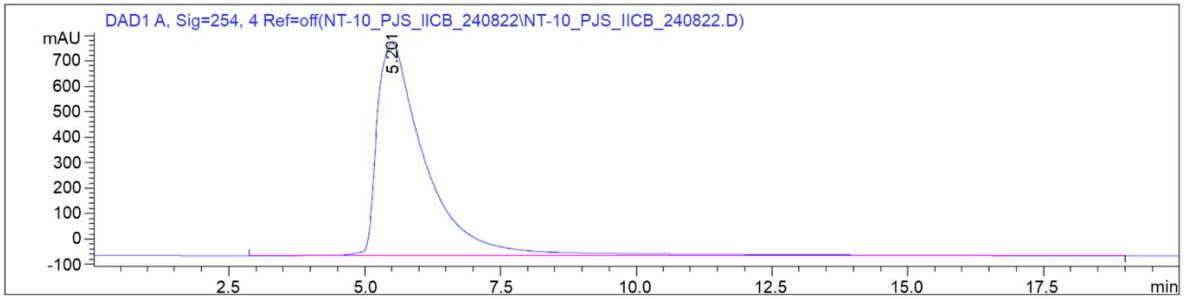
Figure S14. HPLC chromatogram of NT-08 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.156	BB	0.3844	4.46886e4	1668.81836	100.0000
Totals :				4.46886e4	1668.81836	

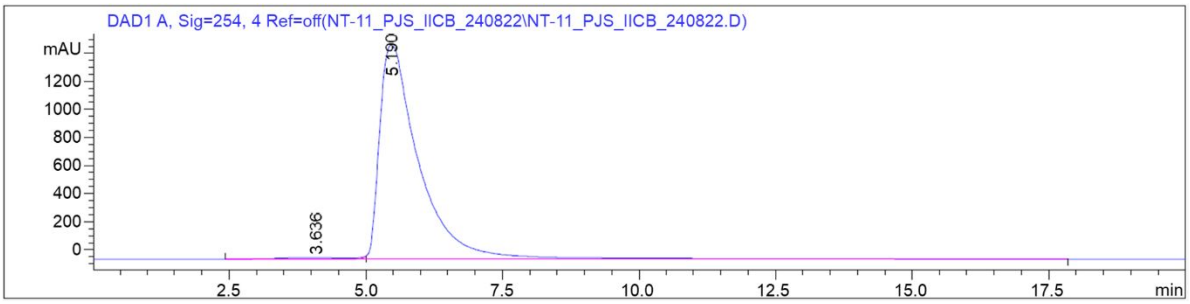
Figure S15. HPLC chromatogram of NT-09 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.201	BB	0.3604	2.10955e4	836.10229	100.0000
Totals :				2.10955e4	836.10229	

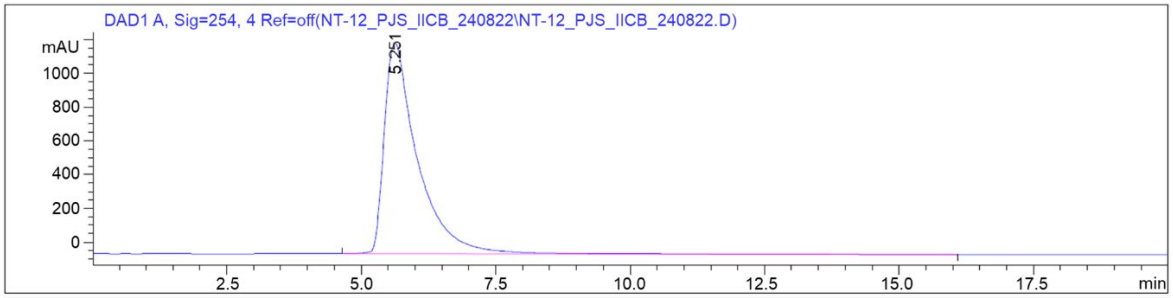
Figure S16. HPLC chromatogram of NT-10 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.636	BV E	0.4779	332.78461	10.49586	1.0668
2	5.190	VB R	0.2892	3.08611e4	1530.61633	98.9332
Totals :				3.11939e4	1541.11219	

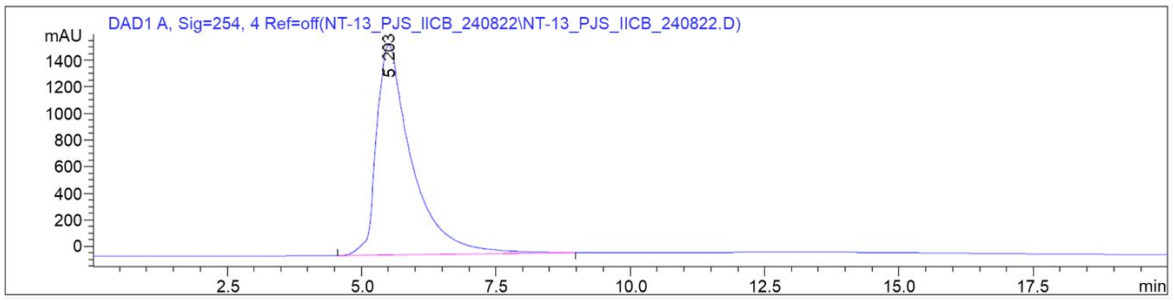
Figure S17. HPLC chromatogram of NT-11 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.251	BB	0.2478	2.16200e4	1250.11133	100.0000
Totals :				2.16200e4	1250.11133	

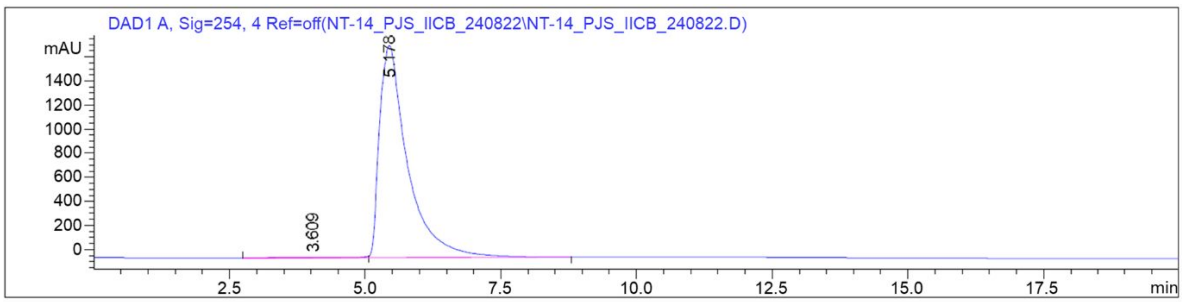
Figure S18. HPLC chromatogram of NT-12 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.203	BB	0.2699	2.90943e4	1587.09729	100.0000
Totals :				2.90943e4	1587.09729	

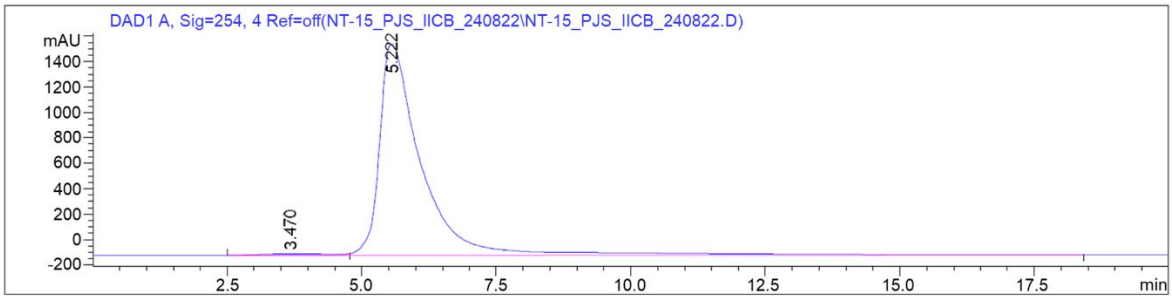
Figure S19. HPLC chromatogram of NT-13 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.609	BV E	0.4782	107.35769	3.20999	0.4200
2	5.178	BB	0.2146	2.54537e4	1761.09973	99.5800
Totals :				2.55611e4	1764.30972	

Figure S20. HPLC chromatogram of NT-14 peptide.



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.470	BV E	0.4457	357.03152	11.46406	1.0175
2	5.222	VB R	0.3103	3.64834e4	1660.83643	98.9825
Totals :				3.68584e4	1672.30049	

Figure S21. HPLC chromatogram of KLVFF peptide.

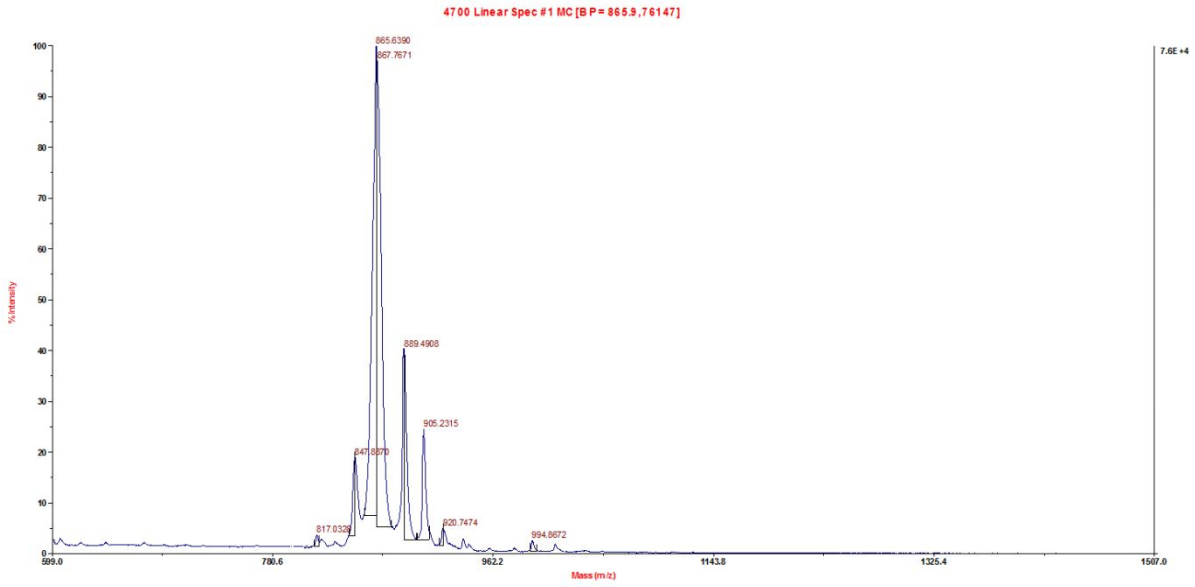


Figure S22. MALDI-mass spectrum of NT-01 (KLLFFAE) expected m/z = 865.5062 and observed m/z = 865.6390.

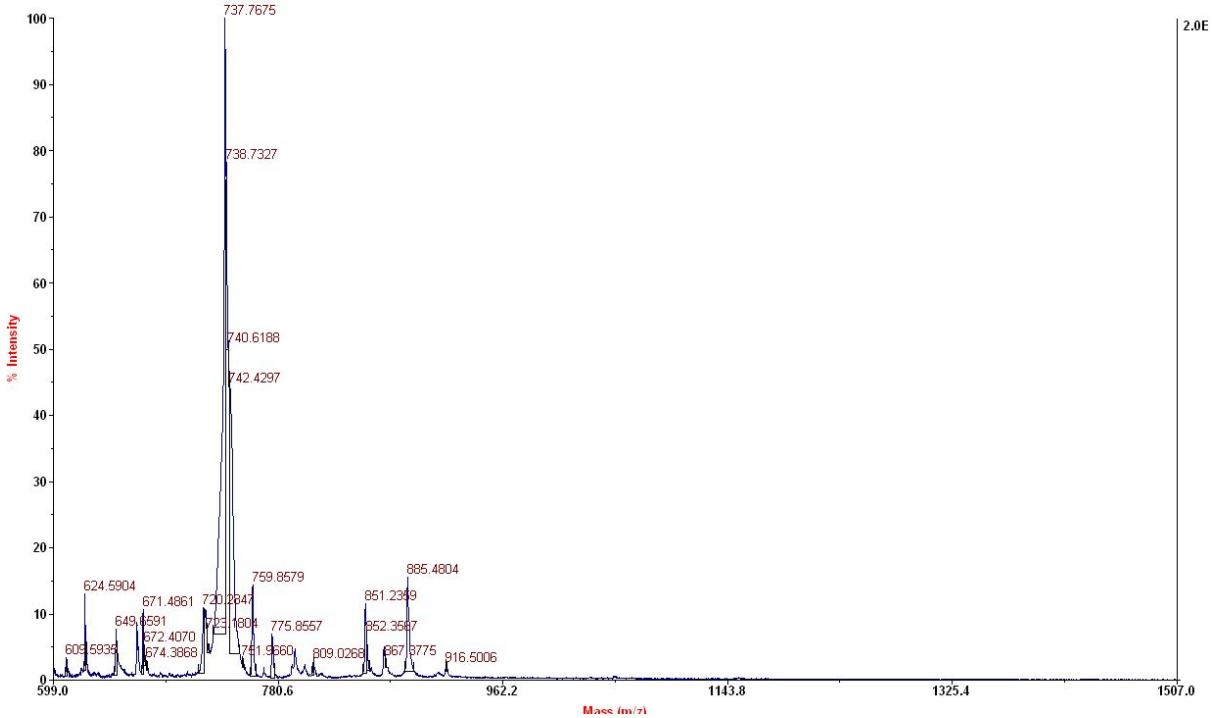


Figure S23. MALDI-mass spectrum of NT-02 (KLLFFA) expected m/z = 736.4636 and observed m+H = 737.7675.

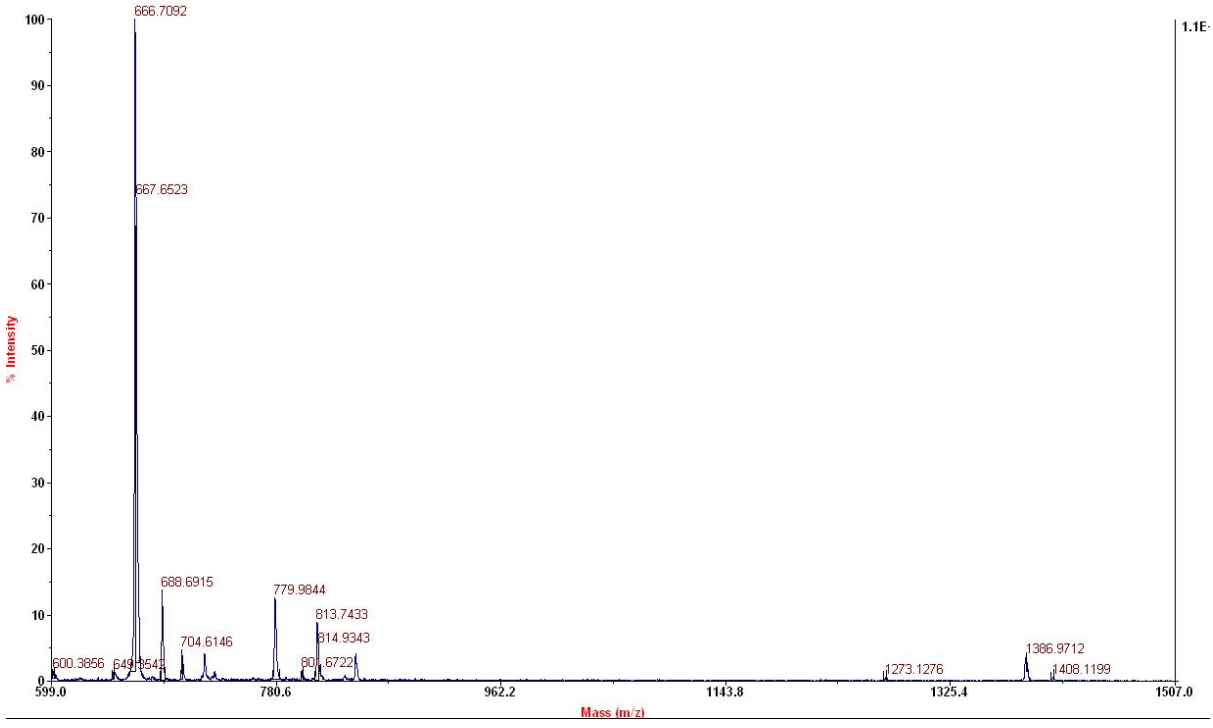


Figure S24. MALDI-mass spectrum of NT-03 (KLLFF) expected m/z = 665.4265 and observed m+H = 666.7092.

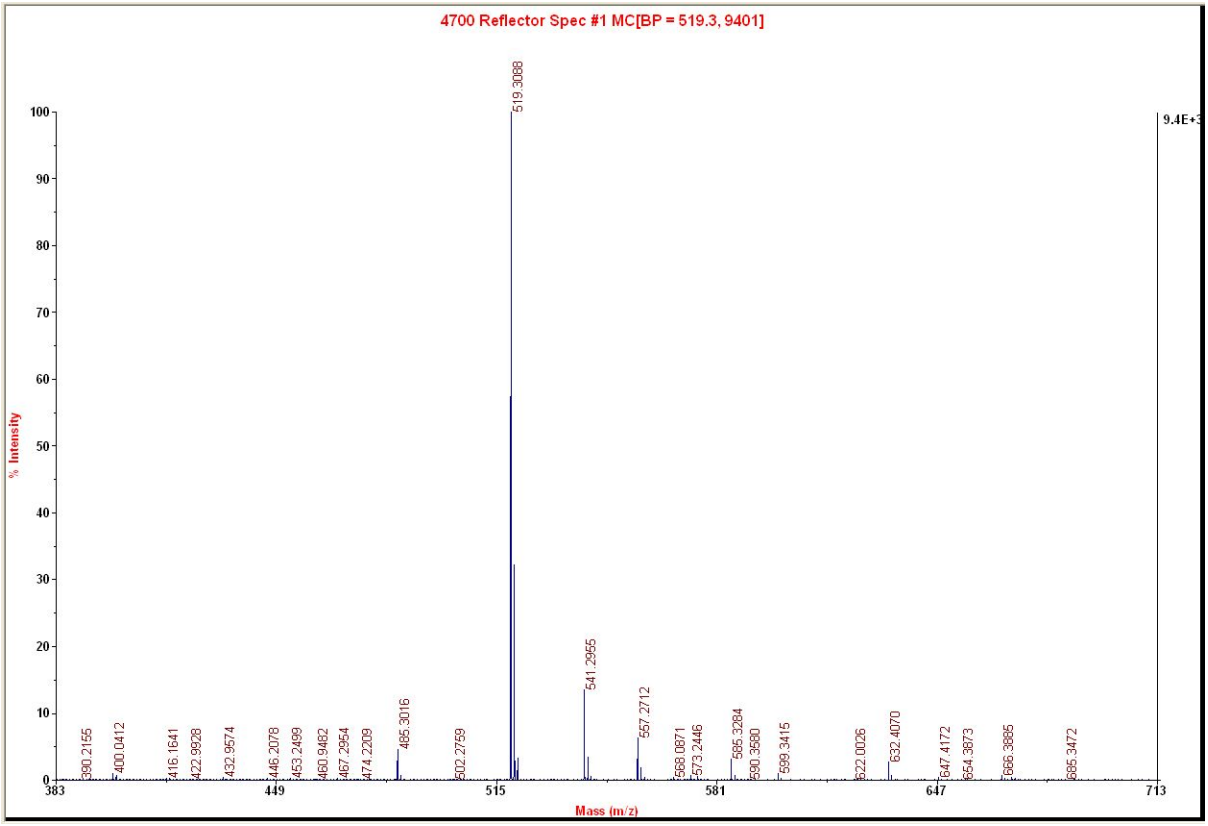


Figure S25. MALDI-mass spectrum of NT-04 (KLLF) expected m/z = 581.3581 and observed m+H = 519.3088.

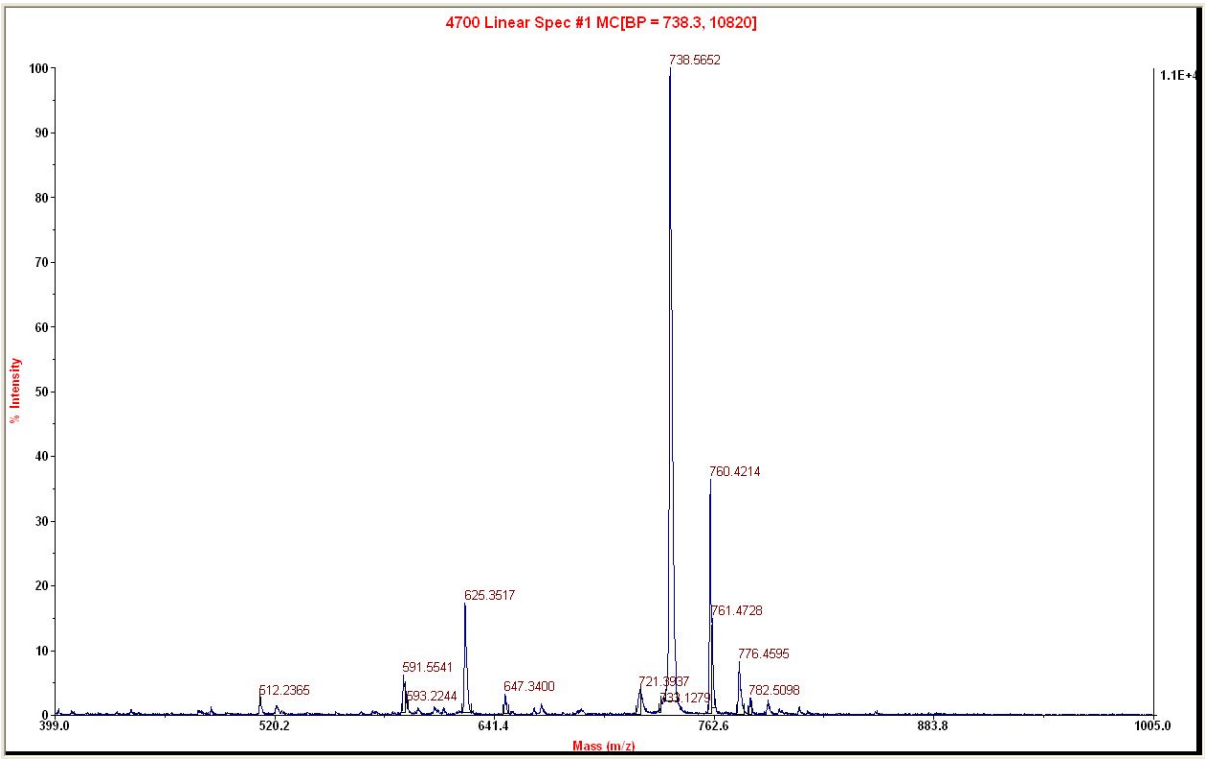


Figure S26. MALDI-mass spectrum of NT-05 (LLFFAE) expected m/z = 737.4112 and observed m+H = 738.5652.

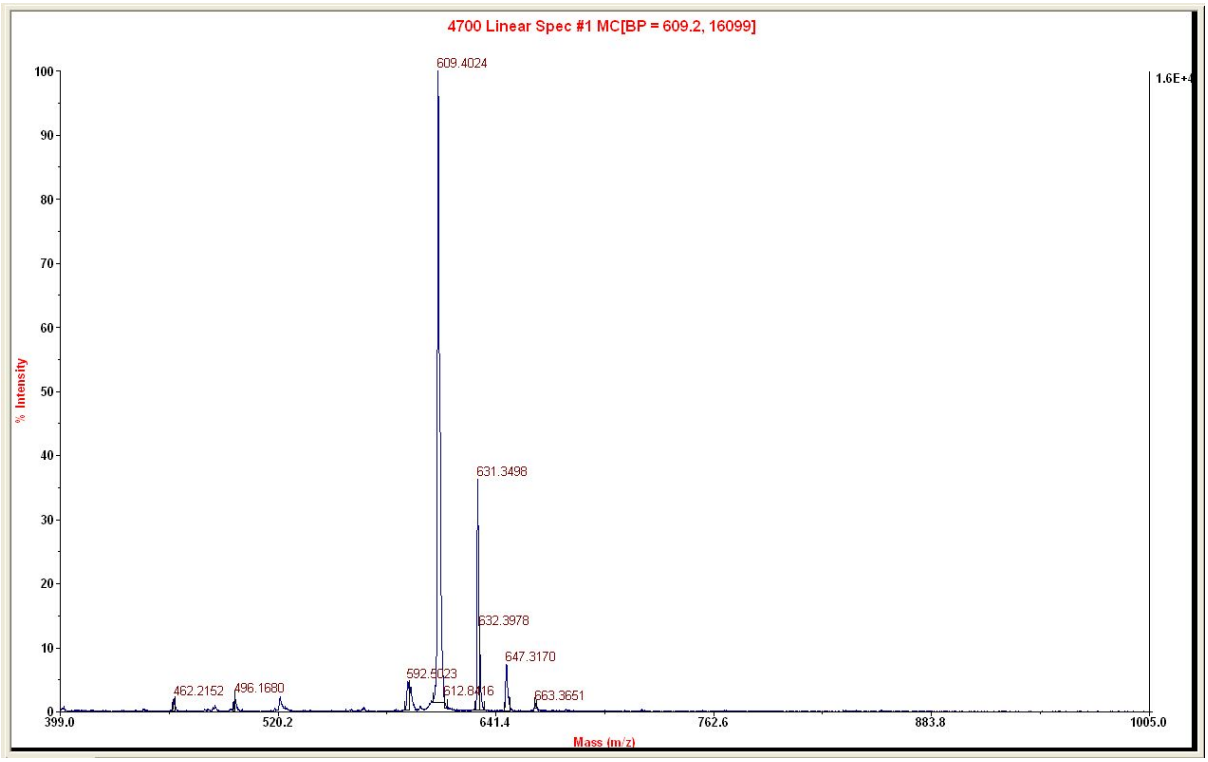


Figure S27. MALDI-mass spectrum of NT-06 (LLFFA) expected m/z = 608.3686 and observed m+H = 609.4024.

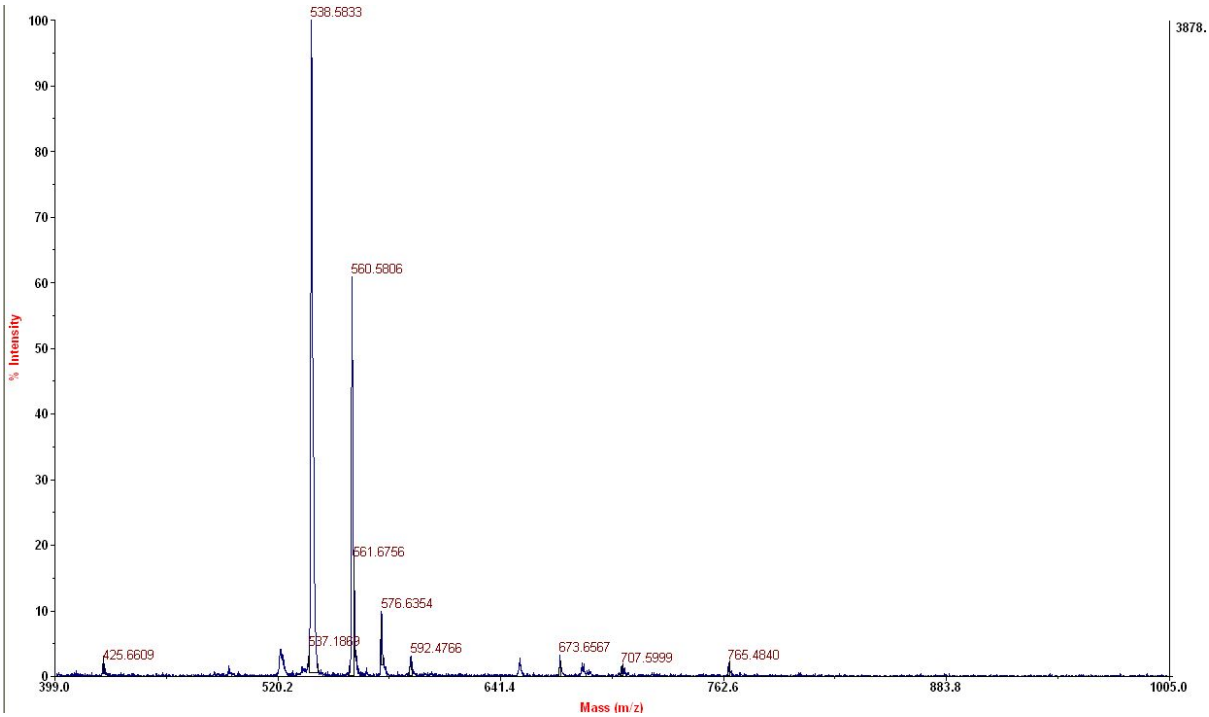


Figure S28. MALDI-mass spectrum of NT-07 (LLFF) expected m/z = 537.3315 and observed m+H = 538.5833.

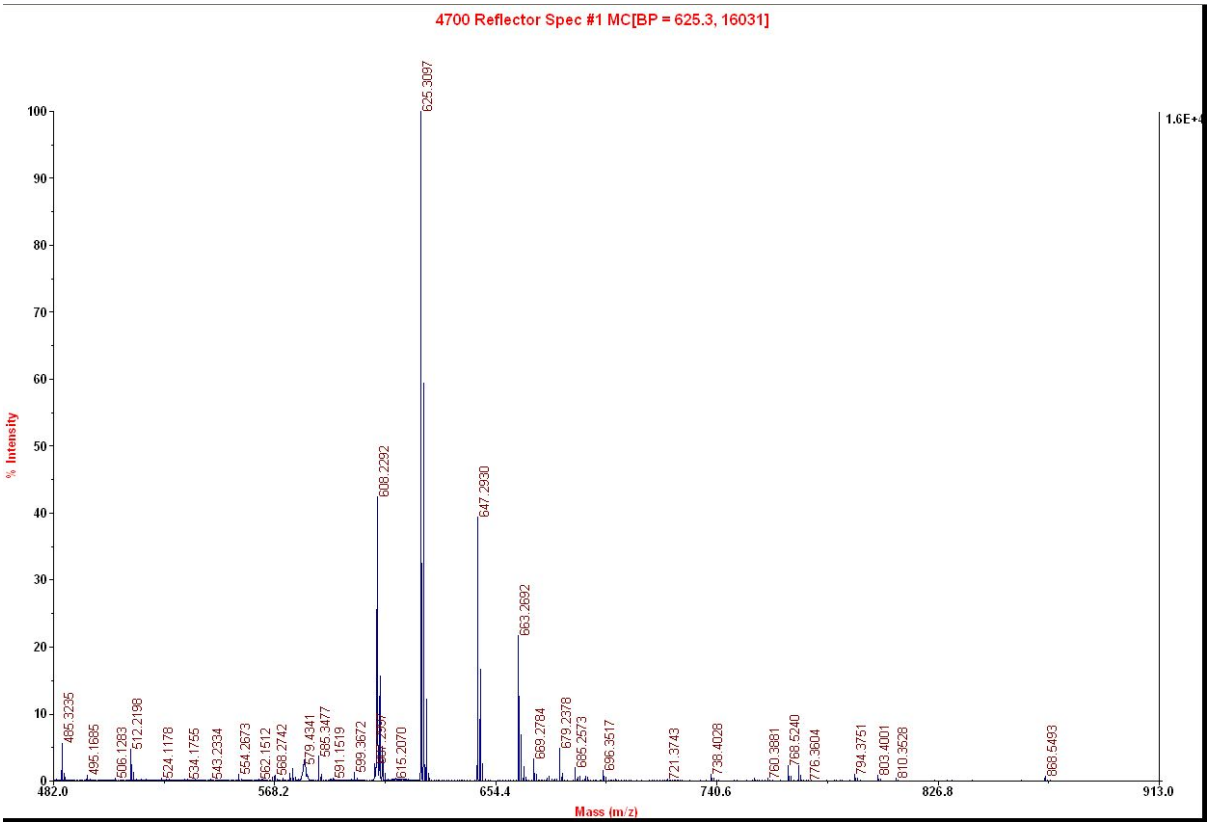


Figure S29. MALDI-mass spectrum of NT-08 (LFFAE) expected m/z = 624.3271 and observed m+H = 625.3097.

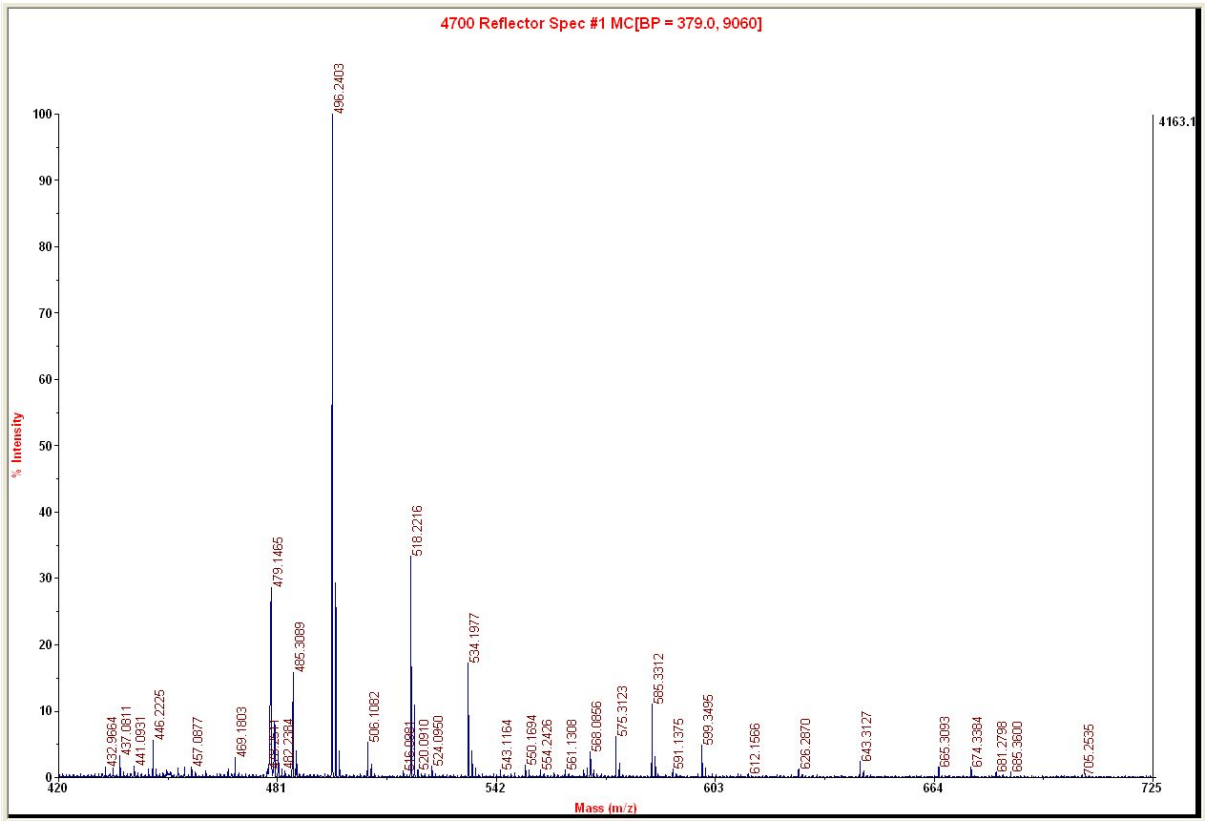


Figure S30. MALDI-mass spectrum of NT-09 (LFFA) expected m/z = 495.2846 and observed m+H = 496.2403.

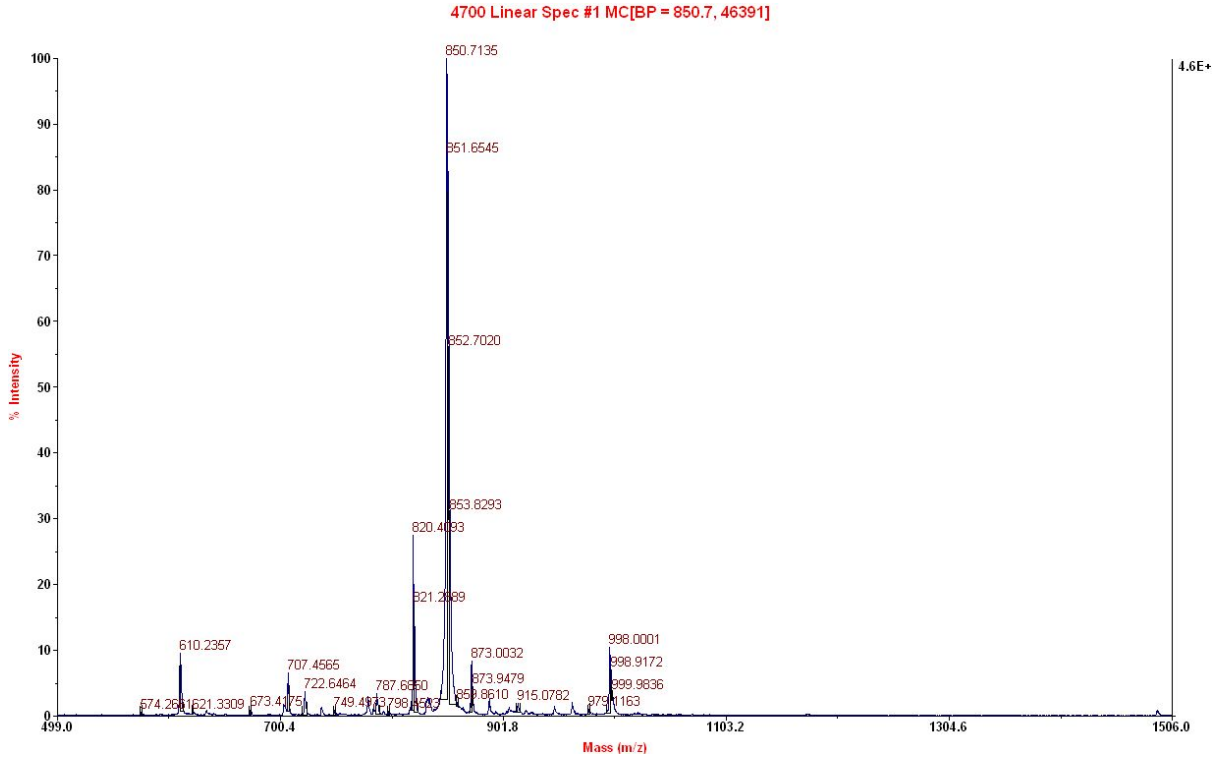


Figure S31. MALDI-mass spectrum of NT-10 (KLPFFAE) expected m/z = 849.4749 and observed m+H = 850.7135.

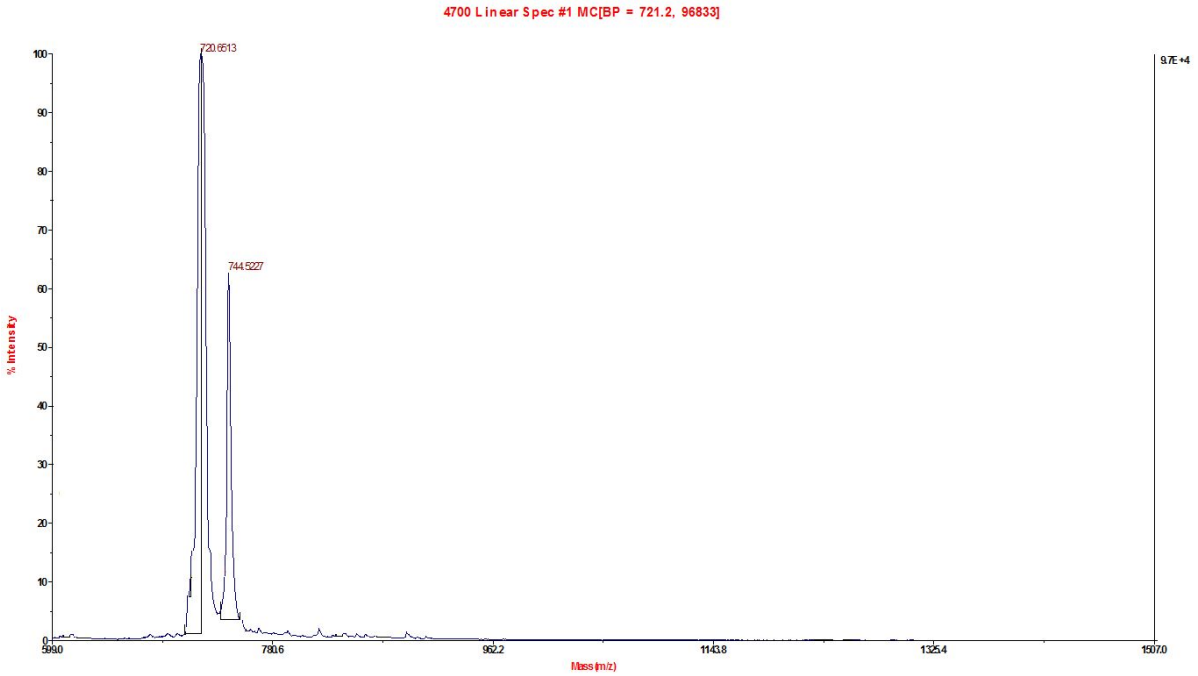


Figure S32. MALDI-mass spectrum of NT-11 KLPFFA expected m/z = 720.4323 and observed m/z = 720.6613.

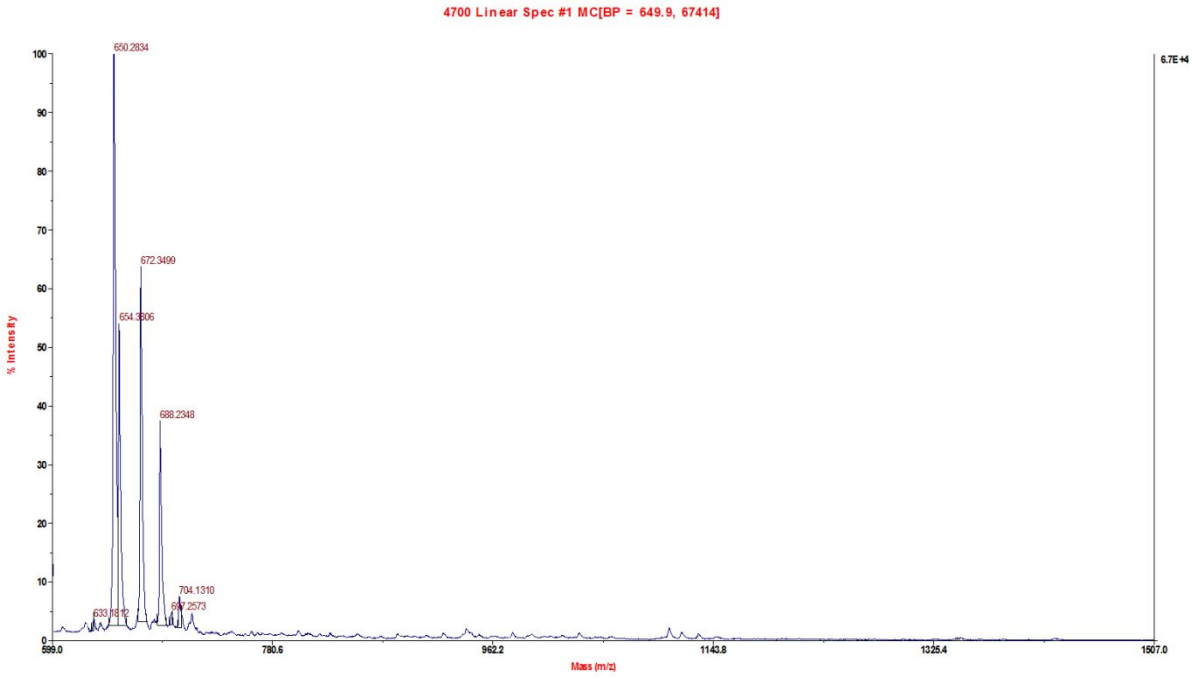


Figure S33. MALDI-mass spectrum of NT-12 KLPFF expected m/z = 649.3952 and observed m+H = 650.2834.

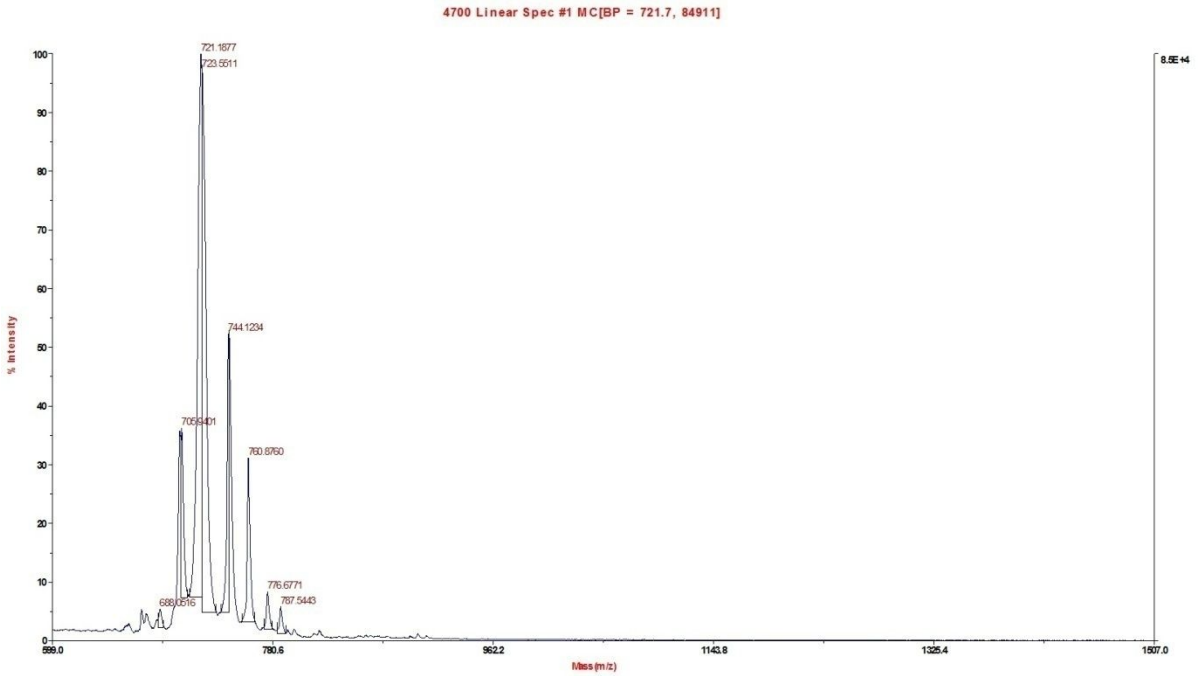


Figure S34. MALDI-mass spectrum of NT-13 LPFFAE expected m/z = 721.3799 and observed m/z = 721.1677

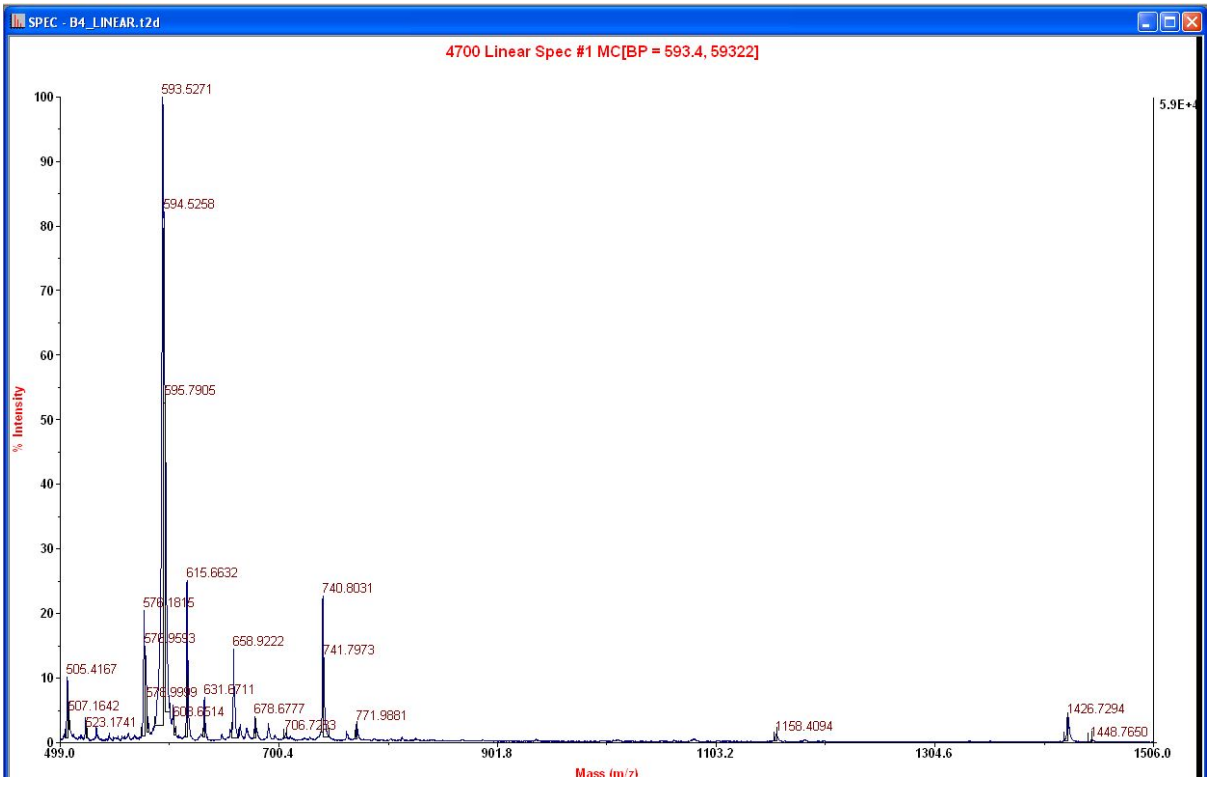


Figure S35. MALDI-mass spectrum of NT-14 KLLFFA expected m/z = 592.3373 and observed m+H = 593.5271.

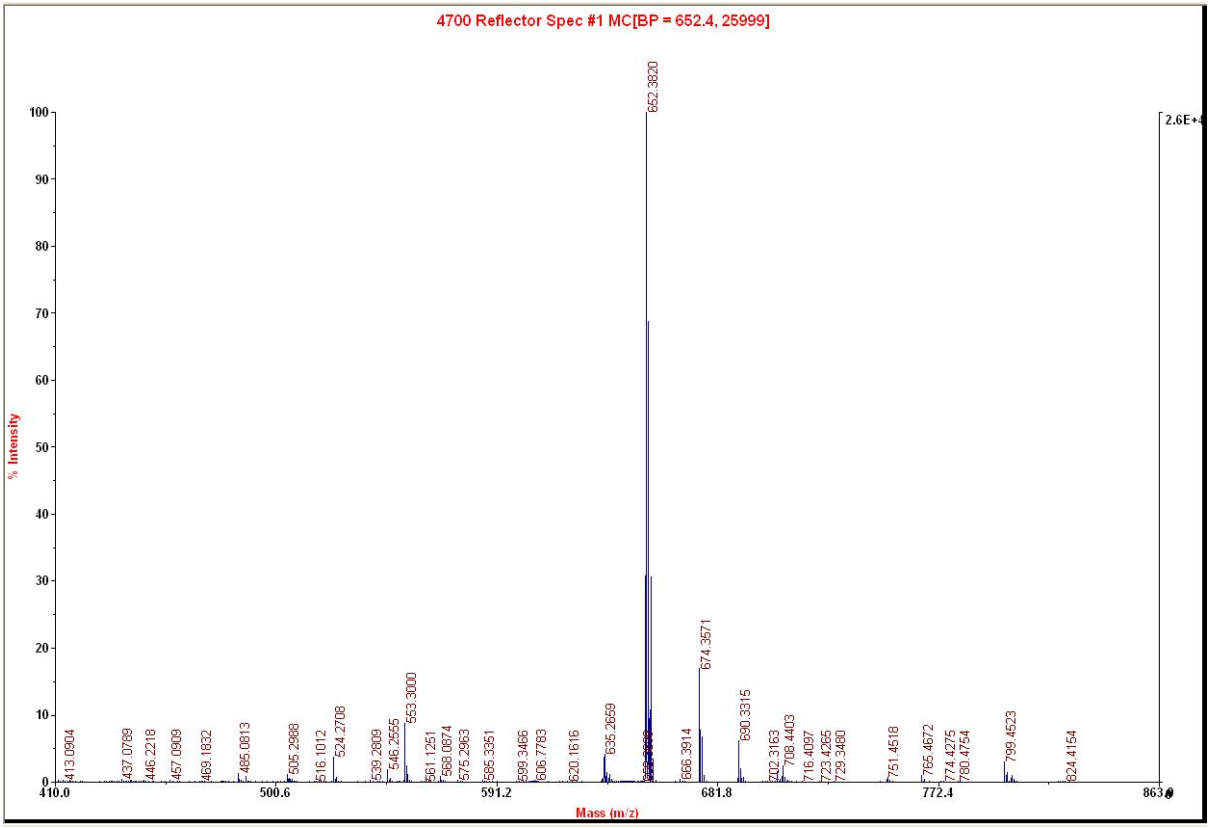


Figure S36. MALDI-mass spectrum of KLVFF expected m/z = 651.4108 and observed m+H = 652.3820.

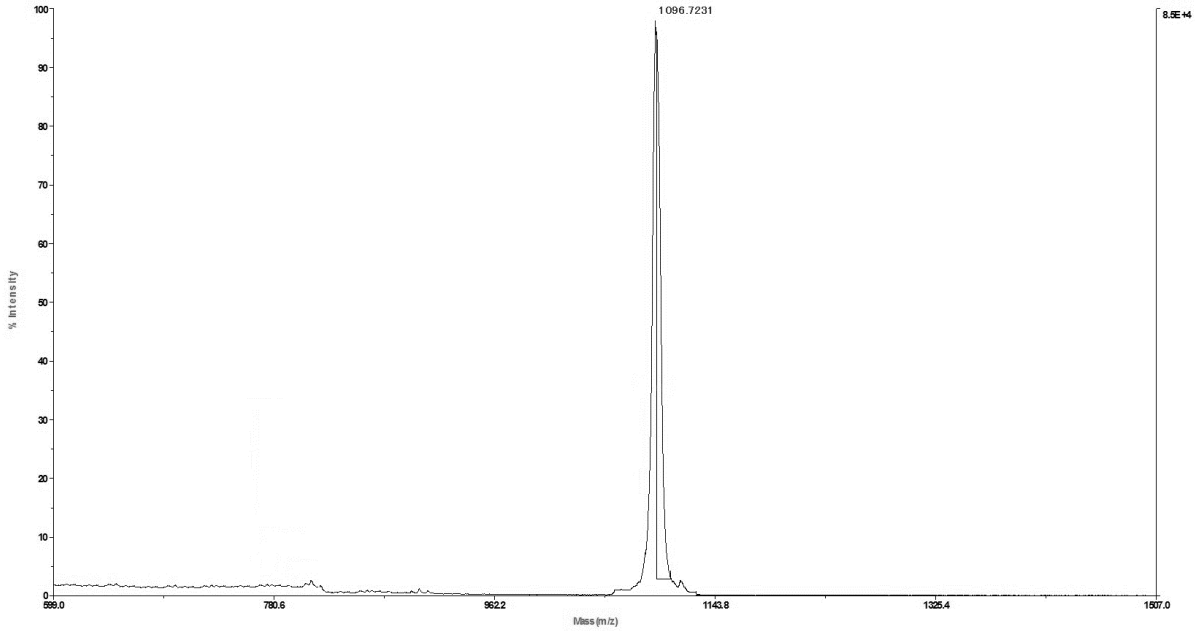


Figure S37. MALDI-mass spectrum of FITC attached NT-02 peptide expected m/z = 1095.4953 and observed m+H = 1096.7231.

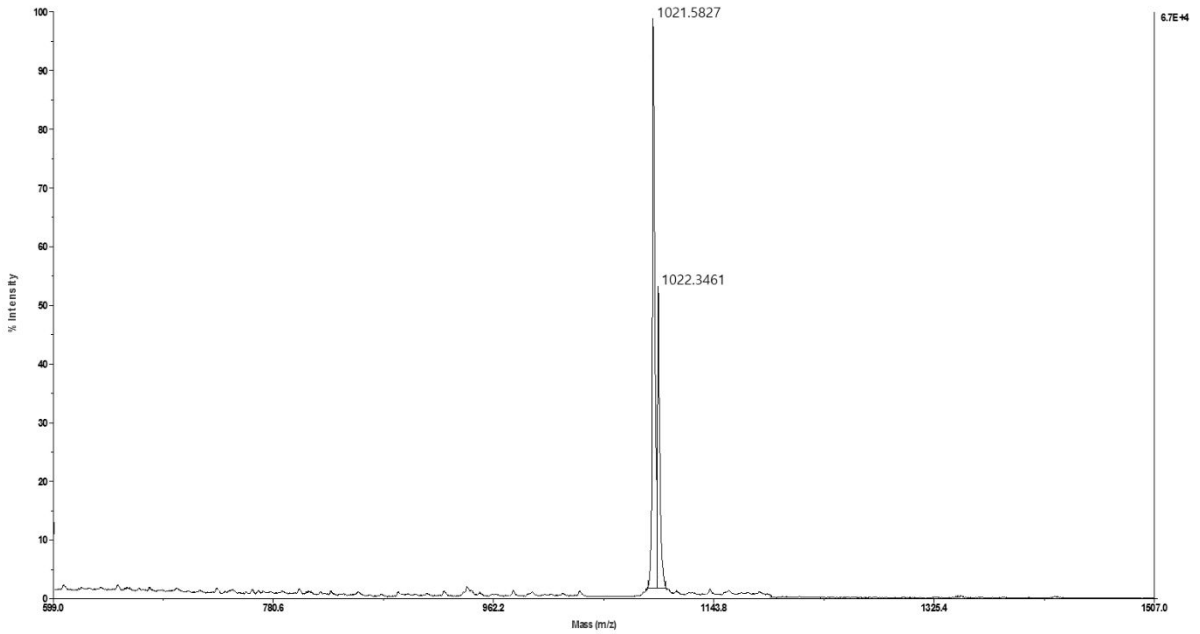


Figure S38. MALDI-mass spectrum of FITC attached NT-03 expected m/z = 1023.4742 and observed m /z = 1022.3461.

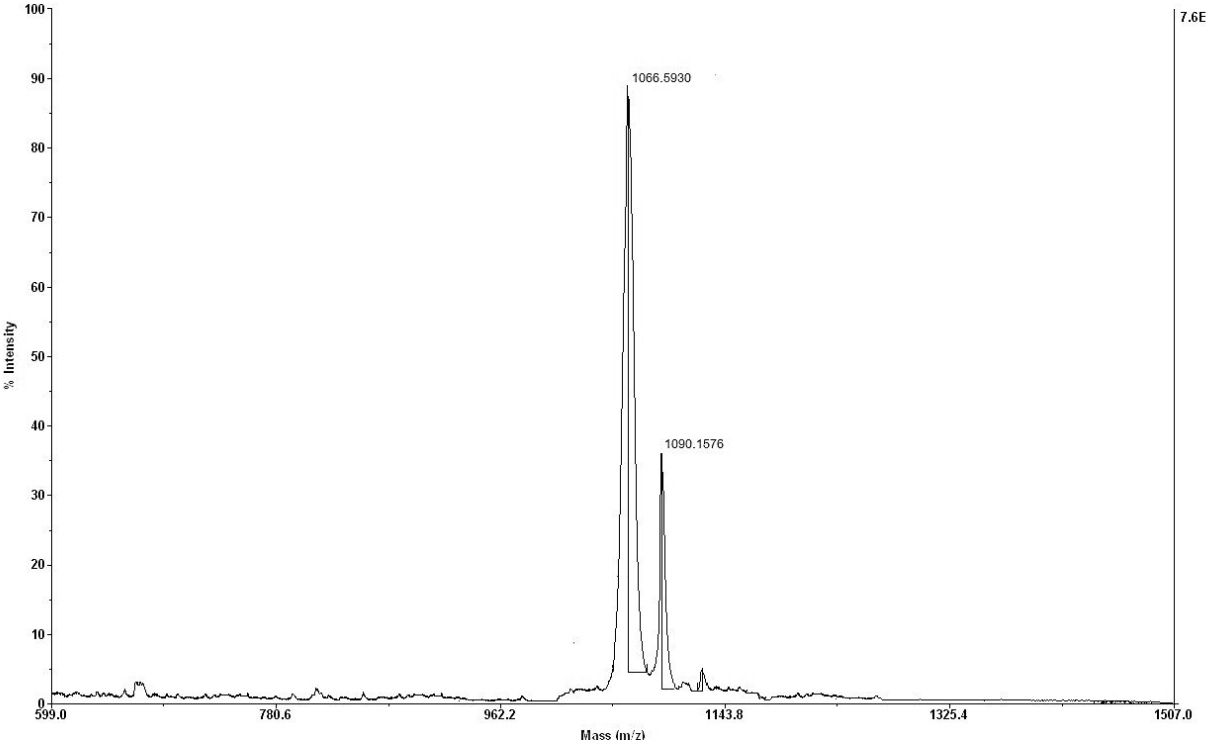


Figure S39. MALDI-mass spectrum of FITC attached NT-13 expected m/z = 1065.4120 and observed m+H = 1066.5930 and m+Na = 1090.1576.

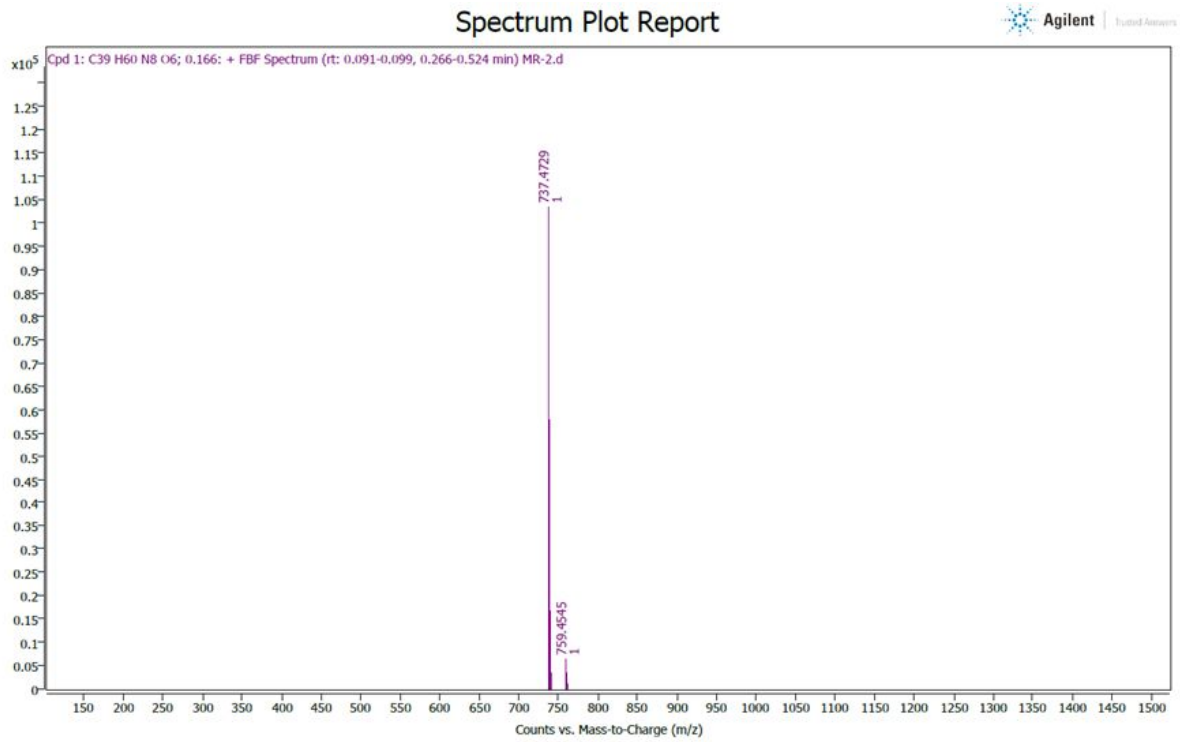


Figure S40. HRMS mass spectrum of NT-02 (KLLFFA) expected m/z = 736.4636 and observed m+H = 737.4729 and m+Na = 759.4545.

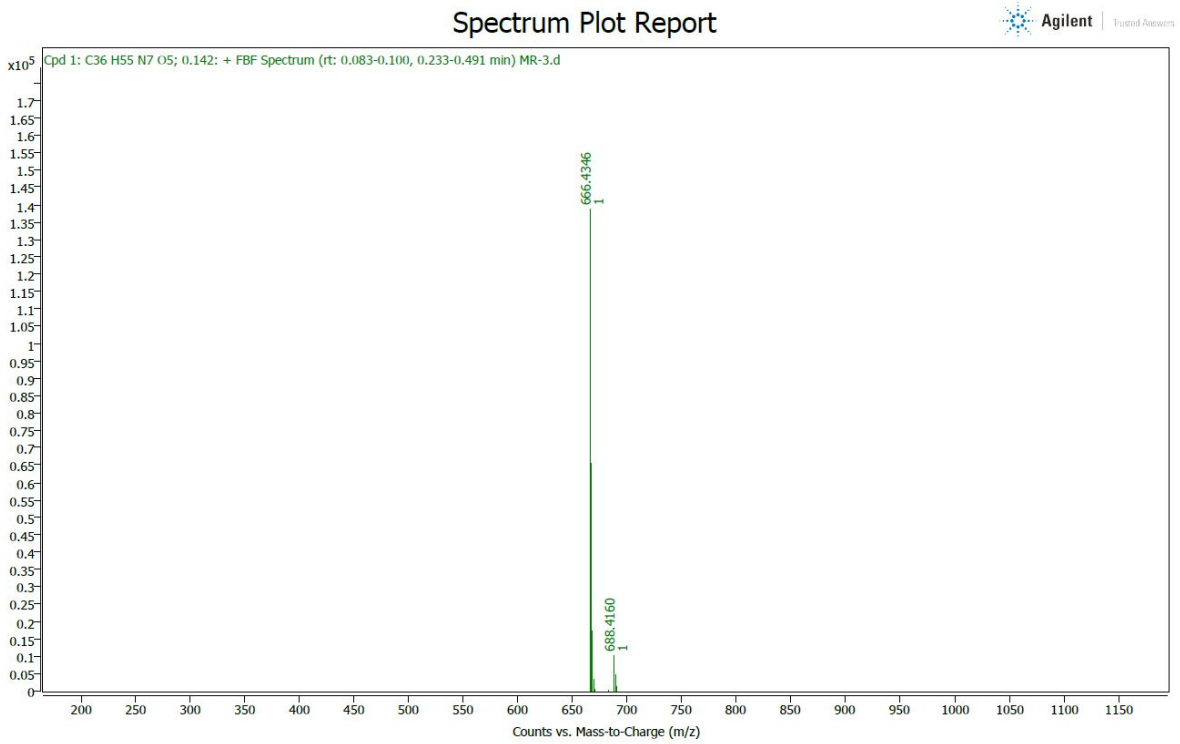


Figure S41. HRMS mass spectrum of NT-03 (KLLFF) expected m/z = 665.2465 and observed m+H = 666.4346 and m+Na = 688.4160.

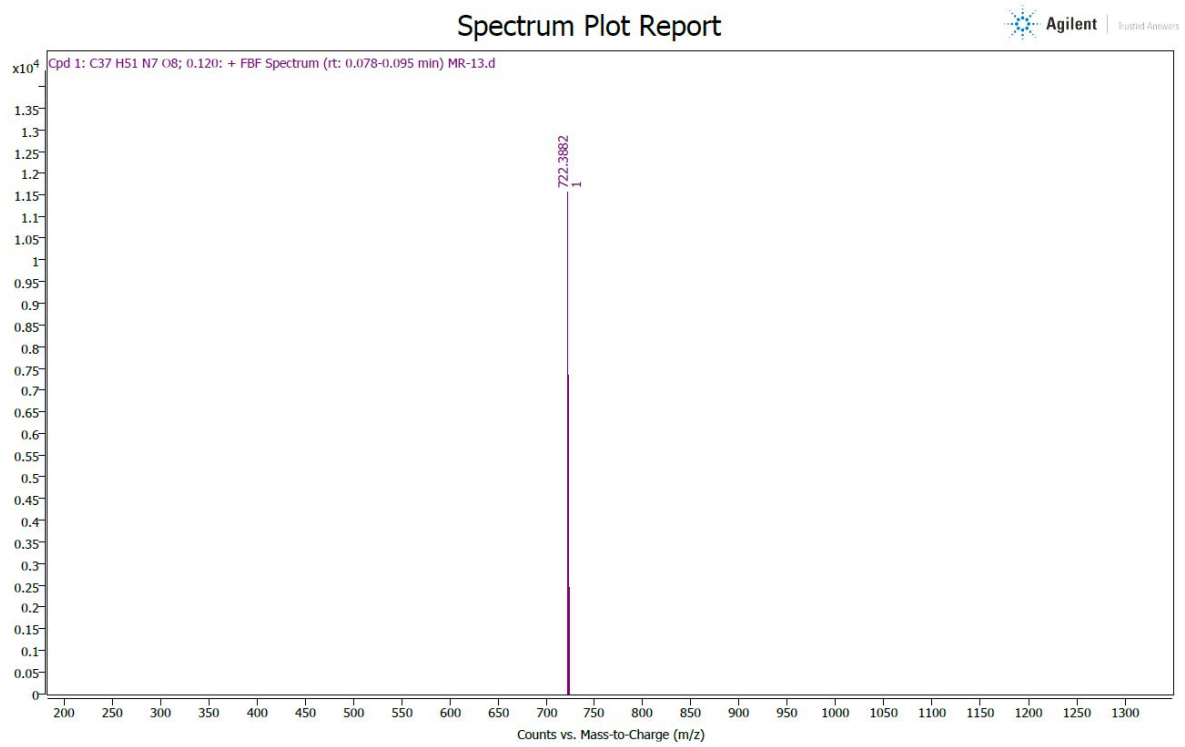


Figure S42. The HRMS mass spectrum of NT-13 (LPFFAE) expected m/z = 721.3799 and observed m+H = 722.3882.

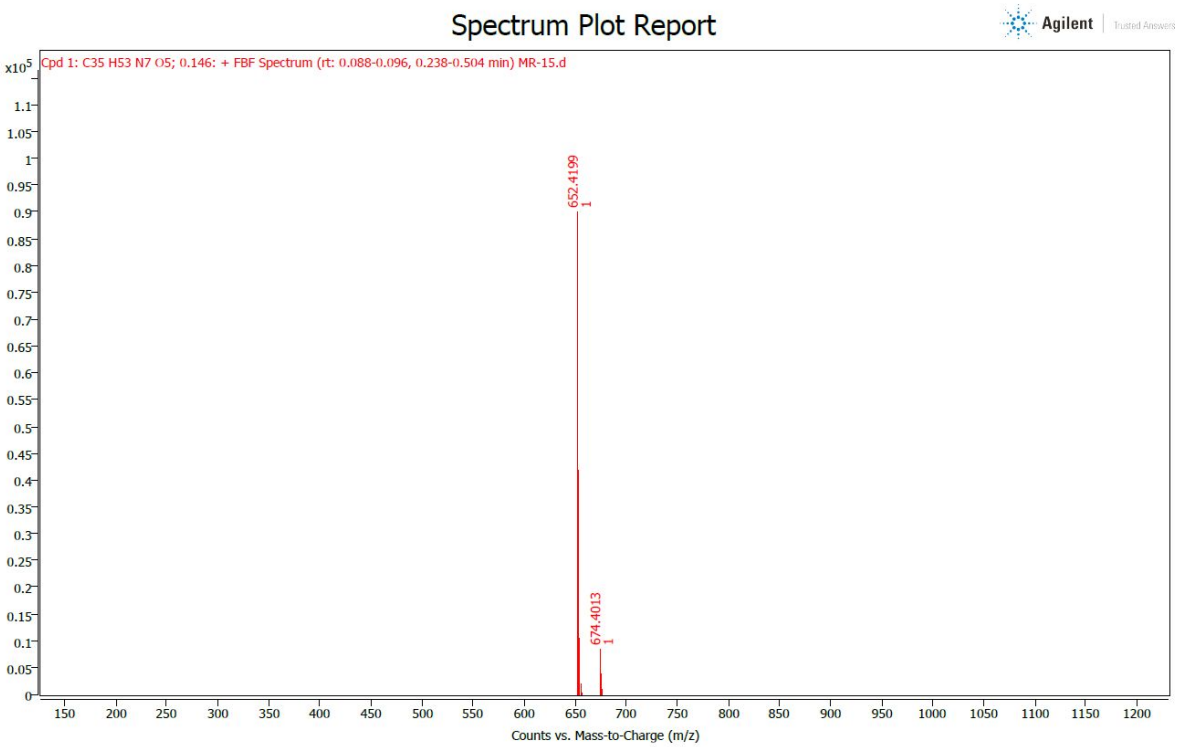


Figure S43. HRMS mass spectrum of KLVFF expected m/z = 651.4108 and observed m+H = 652.4199.