Structural Study of a Peptide Epitope Bearing Multiple Post-Translational Modifications in Rheumatoid Arthritis

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Supplementary Material

Figure S1. Analytical High Performance Liquid Chromatography (HPLC) and Electrospray Mass Spectrometry (ESI-MS) of P1-P11 peptides

Figure S2. CD Spectra of P1-P11 peptides in water. In the legend are indicated the peptides net charge at neutral pH.

Figure S3. The aliphatic and amide regions of the P2 peptide ^{1}H NMR spectra.

Figure S4. The aliphatic and amide regions of the P10 peptide ^{1}H NMR spectra.

Figure S5. The aliphatic and amide regions of the P1 peptide ^{1}H NMR spectra.

Figure S6. Comparison of the amide region of the ^{1}H NMR spectra of the P1, P2 and P10 peptides in a 70:30 (v/v) solution of H_2O/TFE-d2.

Figure S7. (Pages 19 and 20) Selected regions of the 2D NOESY spectrum of P1 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.

Figure S8. (Pages 21 and 22) Selected regions of the 2D NOESY spectrum of P2 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.

Figure S9. (Pages 23 and 24) Selected regions of the 2D NOESY spectrum of P10 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.

Figure S10. Chemical Shift (CS) difference between the experimental (NMR) and calculated CS from the peptide trajectories for the HA and the CA atoms. Sparta+ can only calculate the CS of residues without post-translational modifications, which is why some CS are missing.

Figure S11. Intramolecular contacts arising from the Molecular Dynamics trajectories. The i,i+3 and i,i+4 contacts are typical of α-helices and more prevalent in P10. P2 shows more contacts than P1 because it is more compact, especially in the C-term region. This region is similar to P10 region, as expected because they share the same sequence.

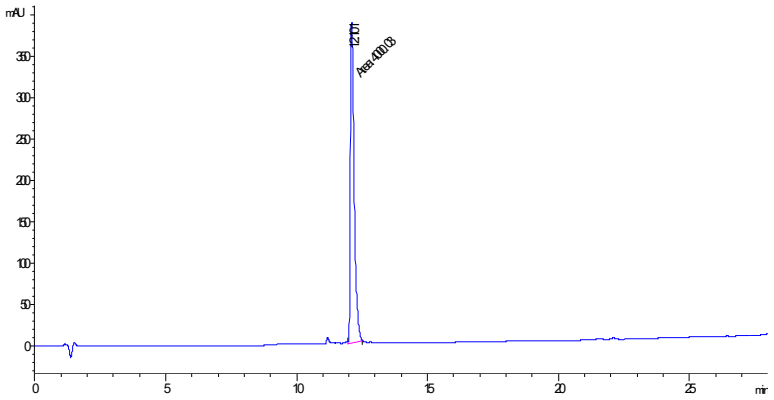
Table S1. Peptides net charge and estimation of the α-helix content according to molar ellipticity at 222nm.

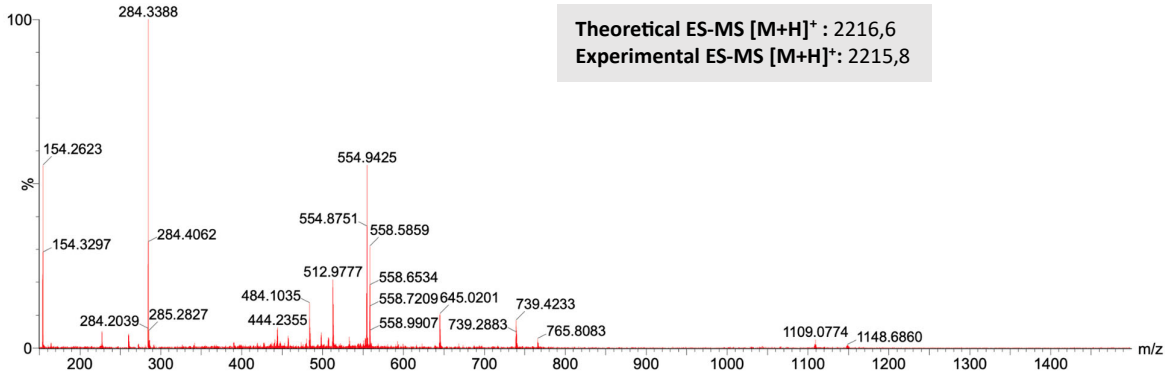
Table S2. P1 peptide NOE restraints in 30% TFE.

Table S3. P2 peptide NOE restraints in 30% TFE.

Table S4. P10 peptide NOE restraints in 30% TFE.

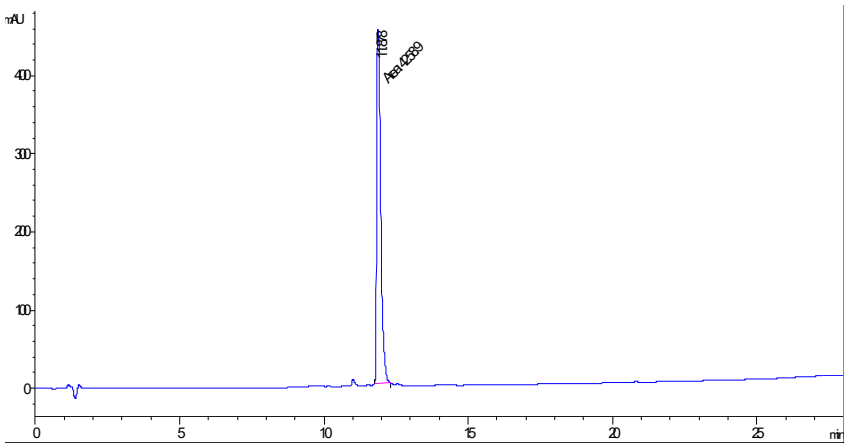
P1

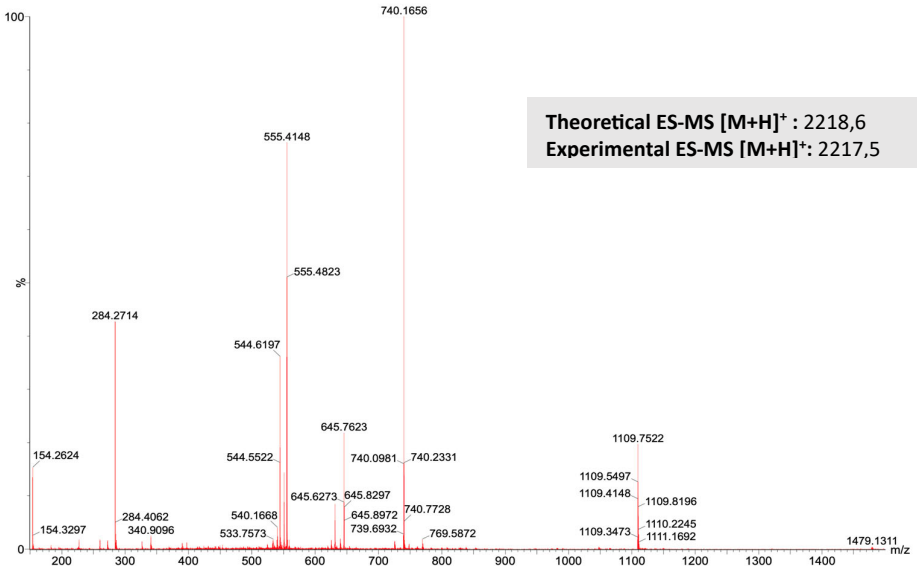




Theoretical ES-MS $[M+H]^+$: 2216,6
Experimental ES-MS $[M+H]^+$: 2215,8

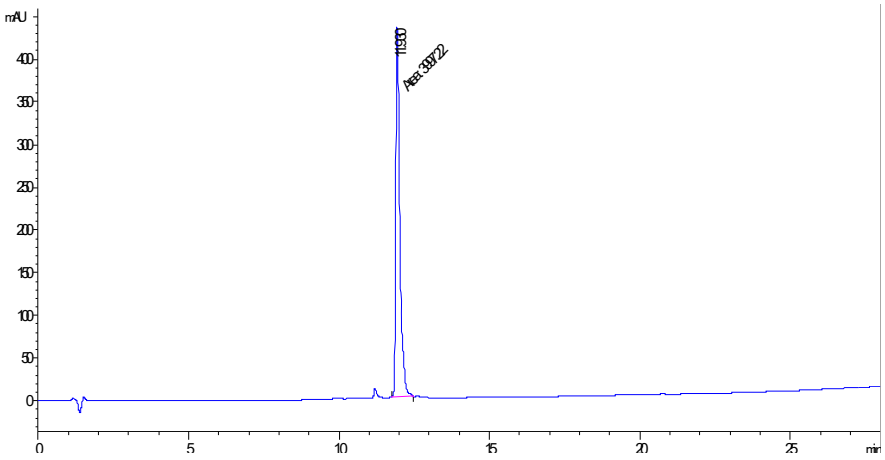
P2

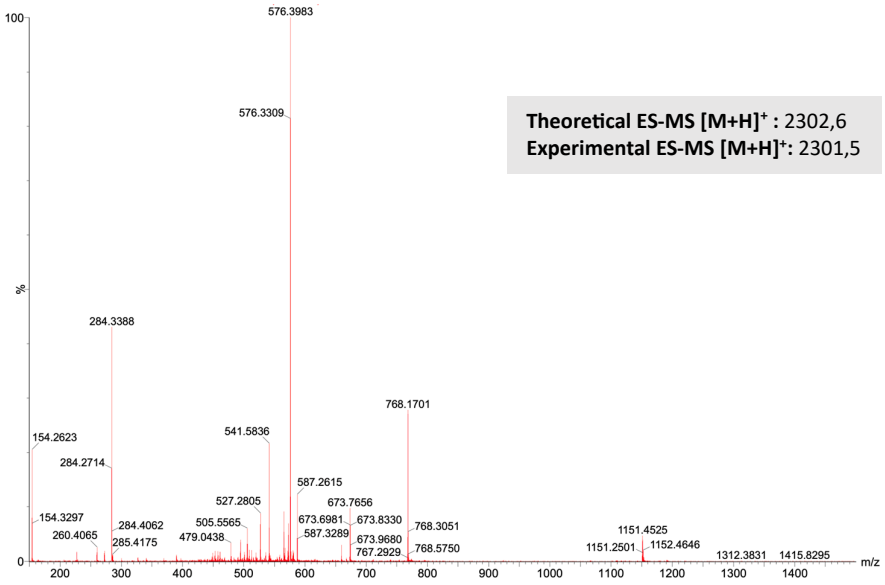




Theoretical ES-MS $[M+H]^+$: 2218,6
Experimental ES-MS $[M+H]^+$: 2217,5

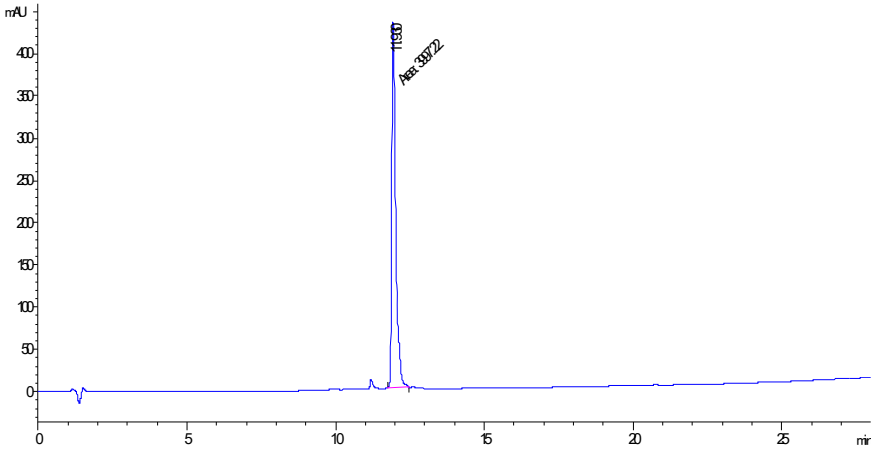
P3

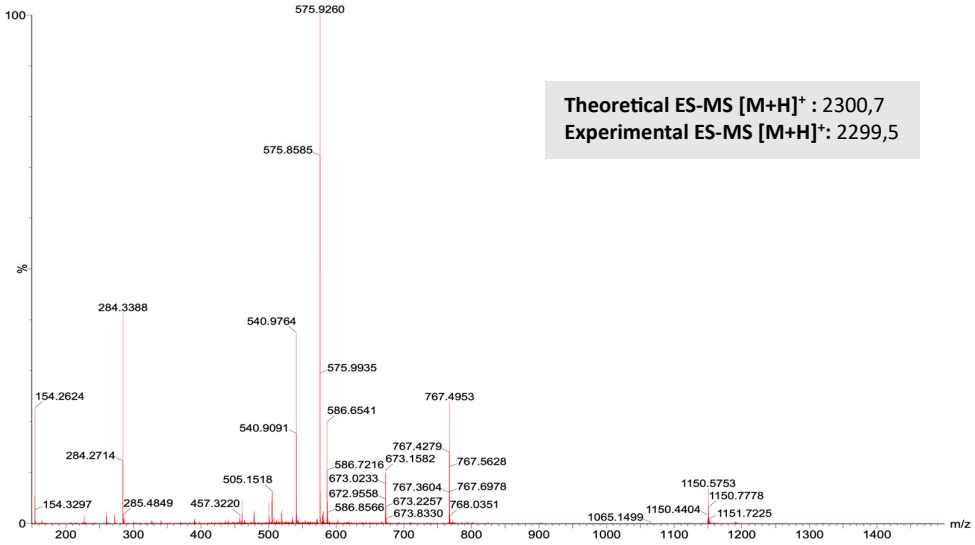




Theoretical ES-MS $[M+H]^+$: 2302,6
Experimental ES-MS $[M+H]^+$: 2301,5

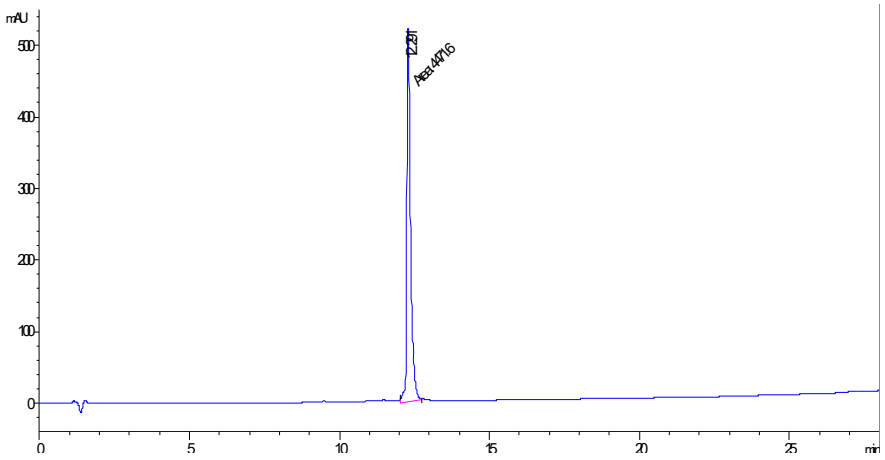
P4

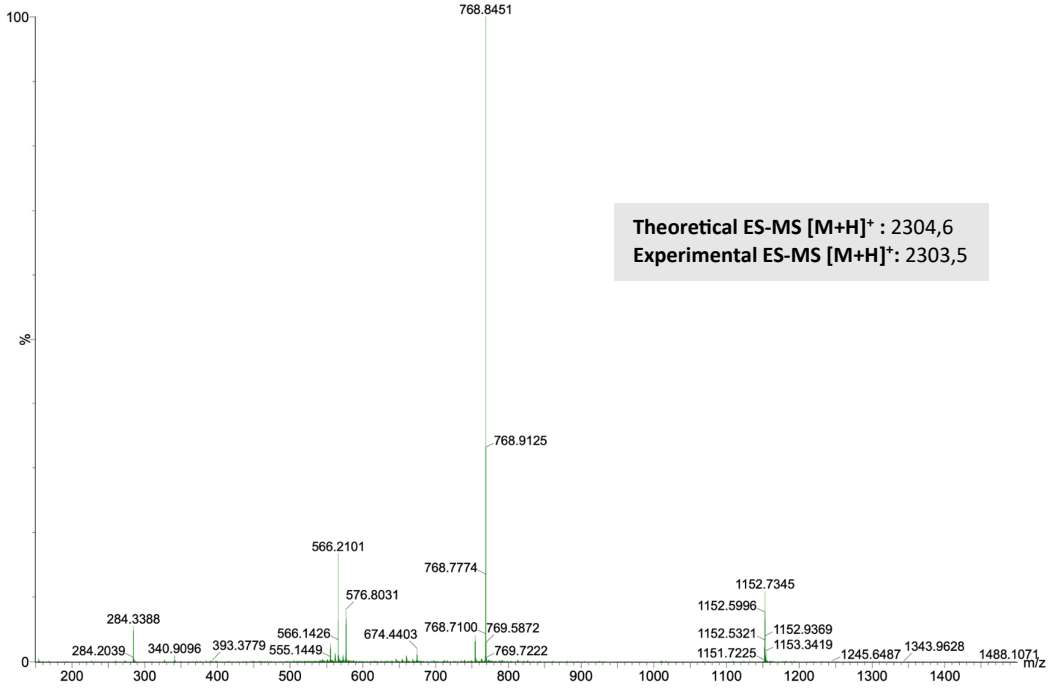




Theoretical ES-MS $[M+H]^+$: 2300,7
Experimental ES-MS $[M+H]^+$: 2299,5

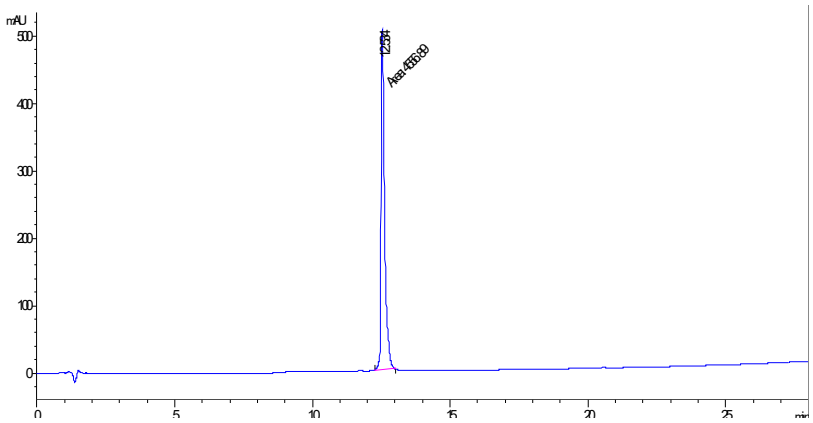
P5

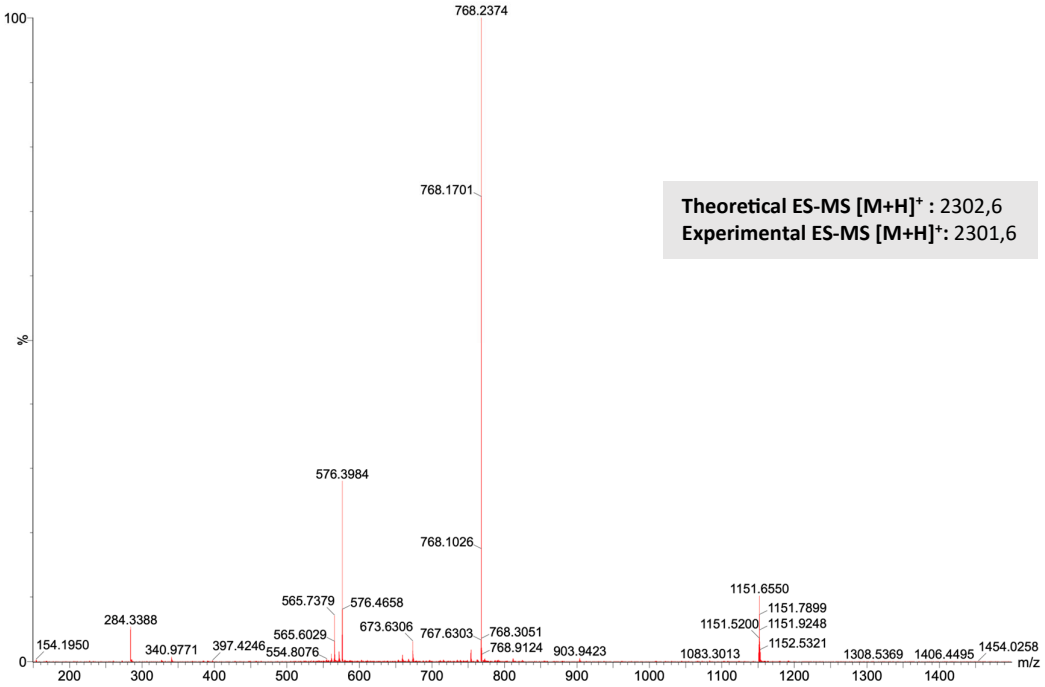




Theoretical ES-MS $[M+H]^+$: 2304,6
Experimental ES-MS $[M+H]^+$: 2303,5

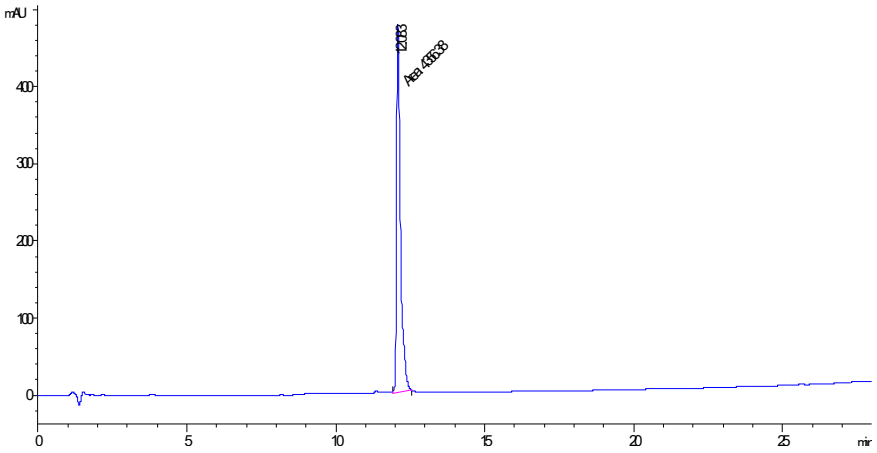
P6

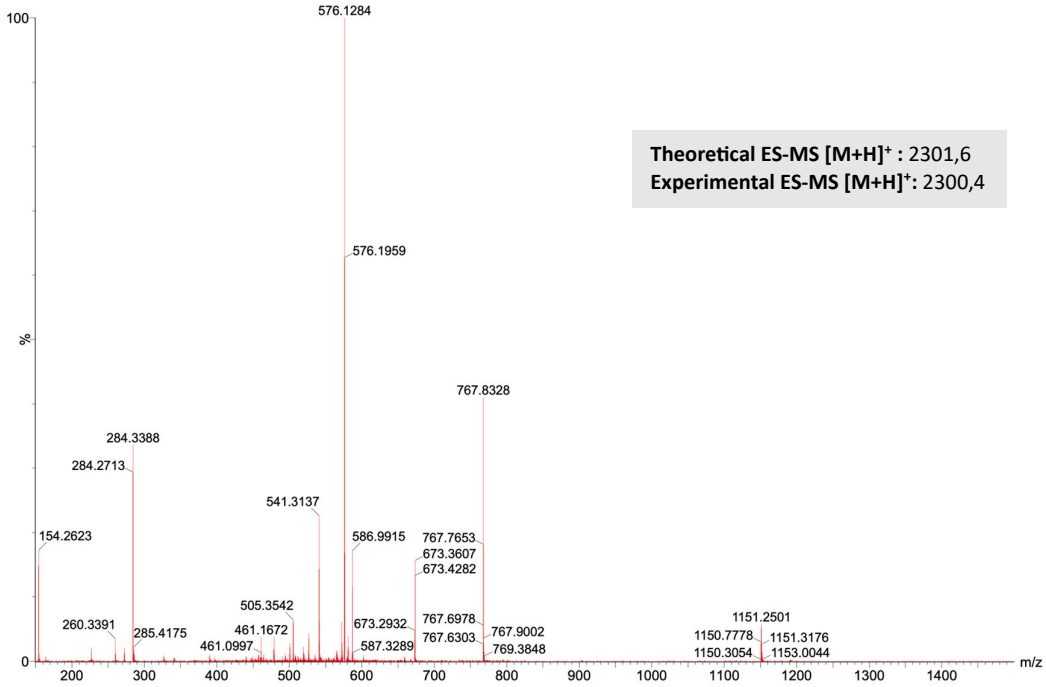




Theoretical ES-MS $[M+H]^+$: 2302,6
Experimental ES-MS $[M+H]^+$: 2301,6

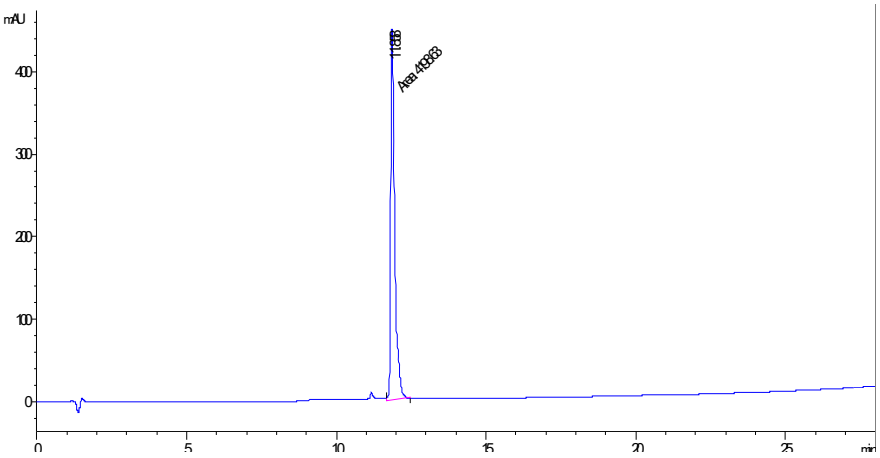
P7

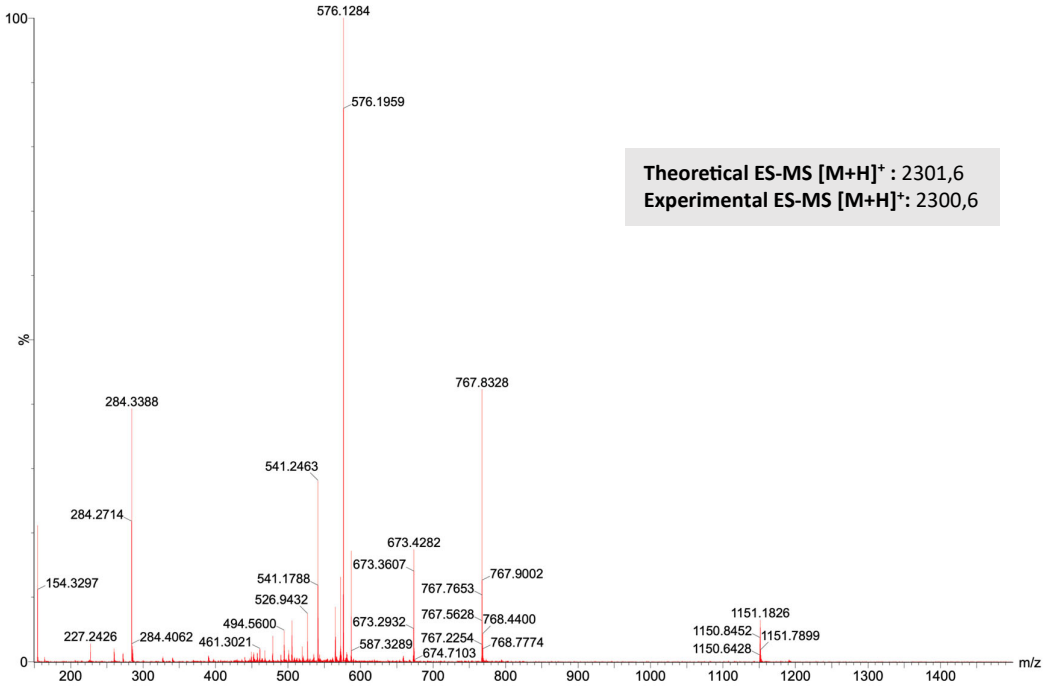




Theoretical ES-MS $[M+H]^+$: 2301,6
Experimental ES-MS $[M+H]^+$: 2300,4

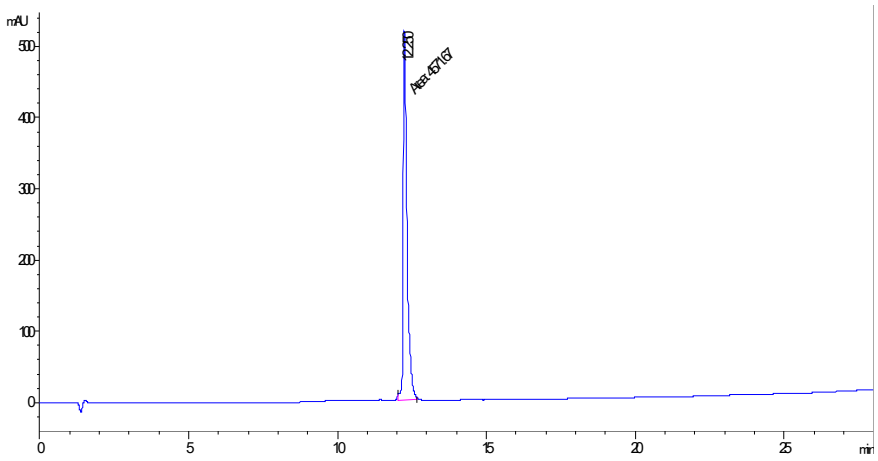
P8

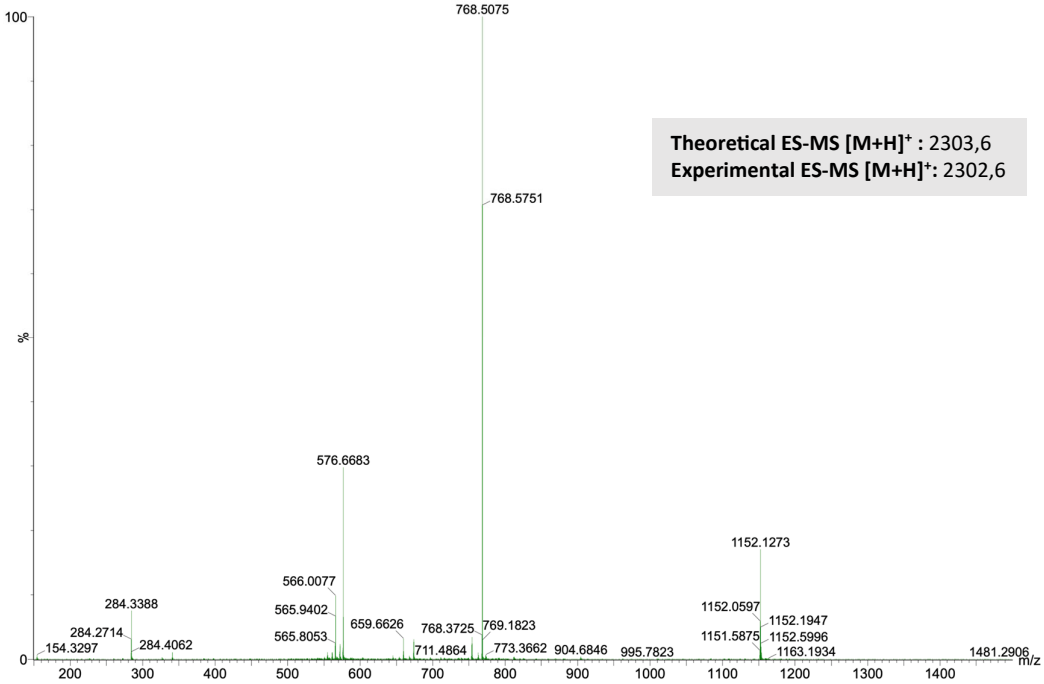




Theoretical ES-MS $[M+H]^+$: 2301,6
Experimental ES-MS $[M+H]^+$: 2300,6

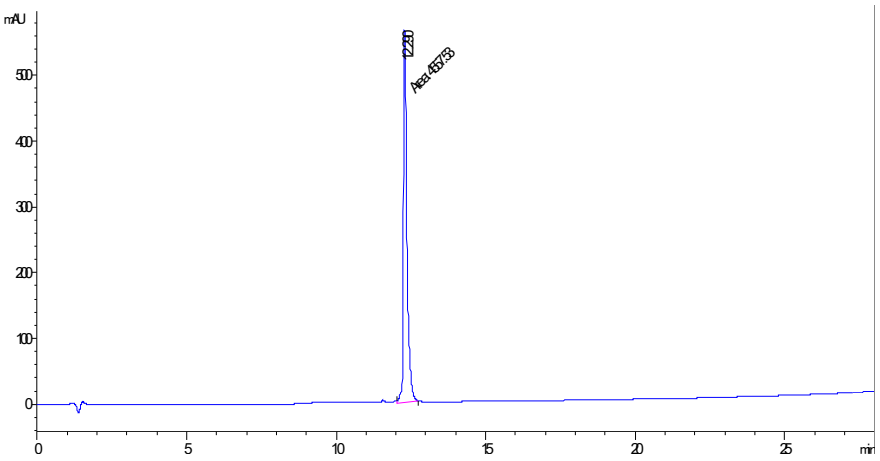
P9

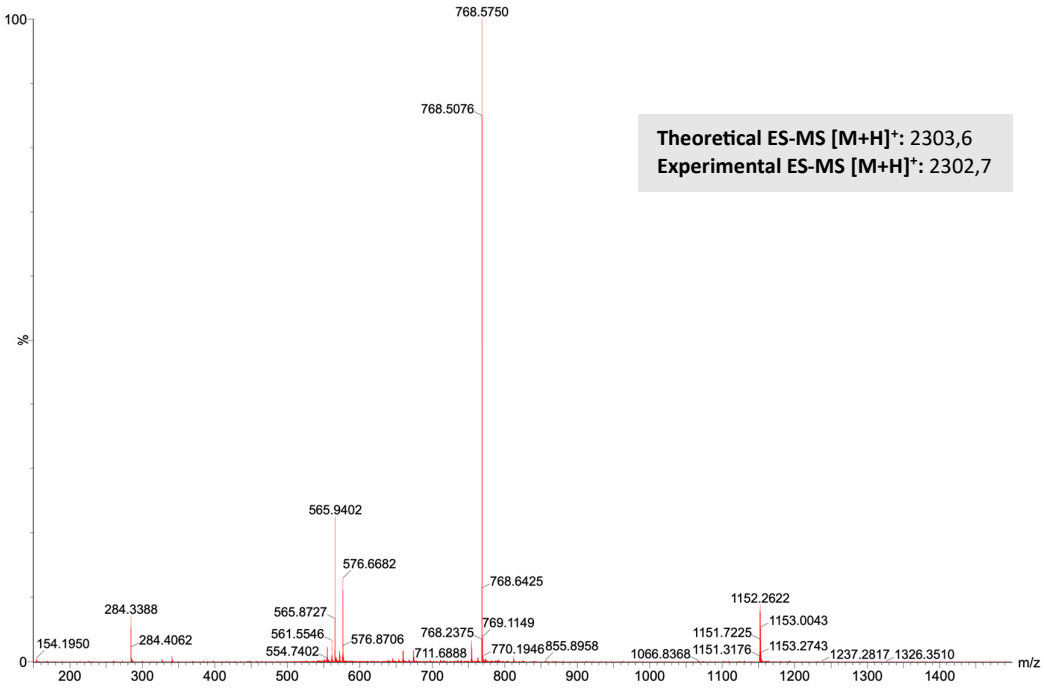




Theoretical ES-MS $[M+H]^+$: 2303,6
Experimental ES-MS $[M+H]^+$: 2302,6

P10





Theoretical ES-MS $[M+H]^+$: 2303,6
Experimental ES-MS $[M+H]^+$: 2302,7

P11

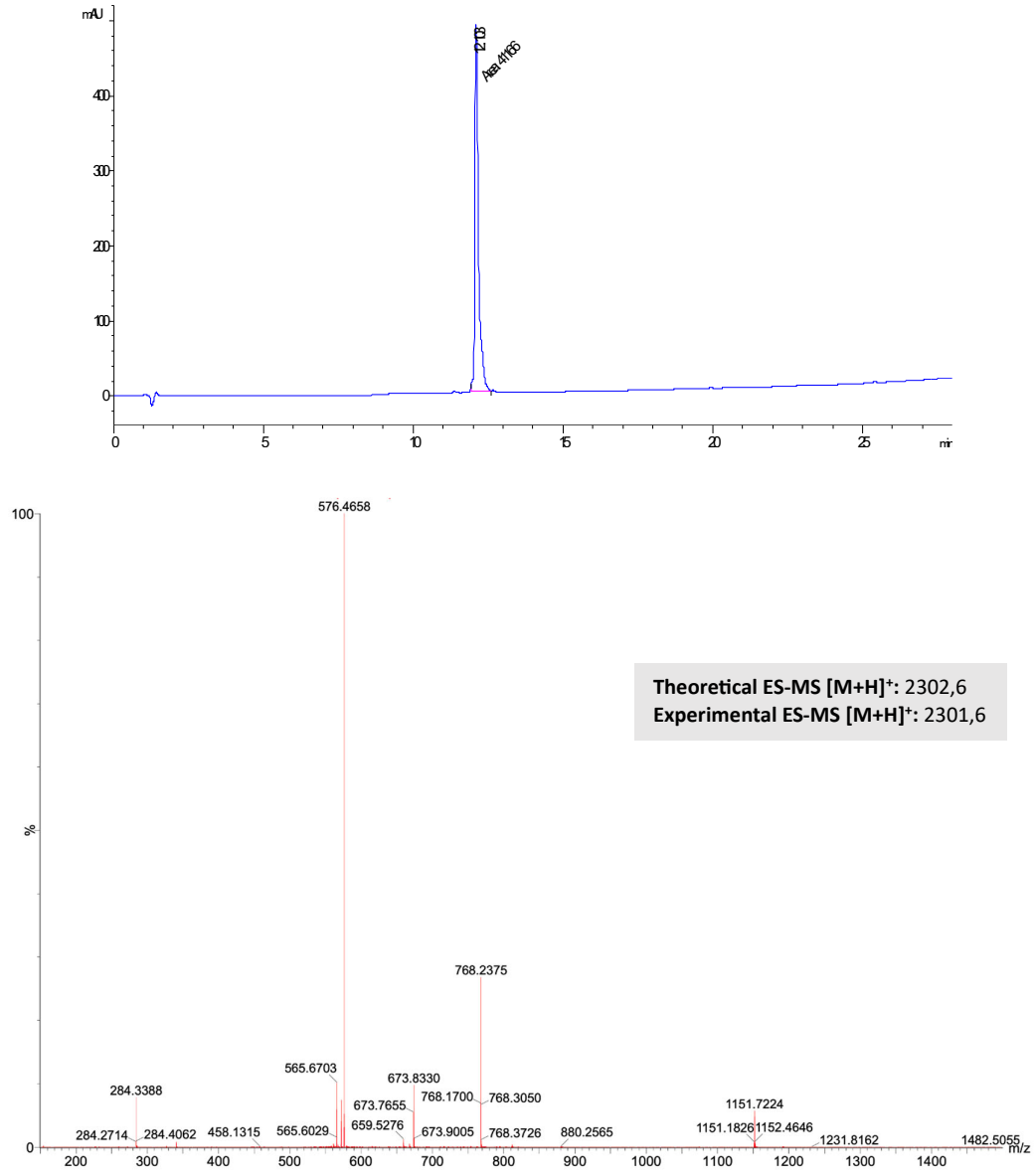


Figure S1. Analytical High Performance Liquid Chromatography (HPLC) and Electrospray Mass Spectrometry (ESI-MS) of P1-P11 peptides

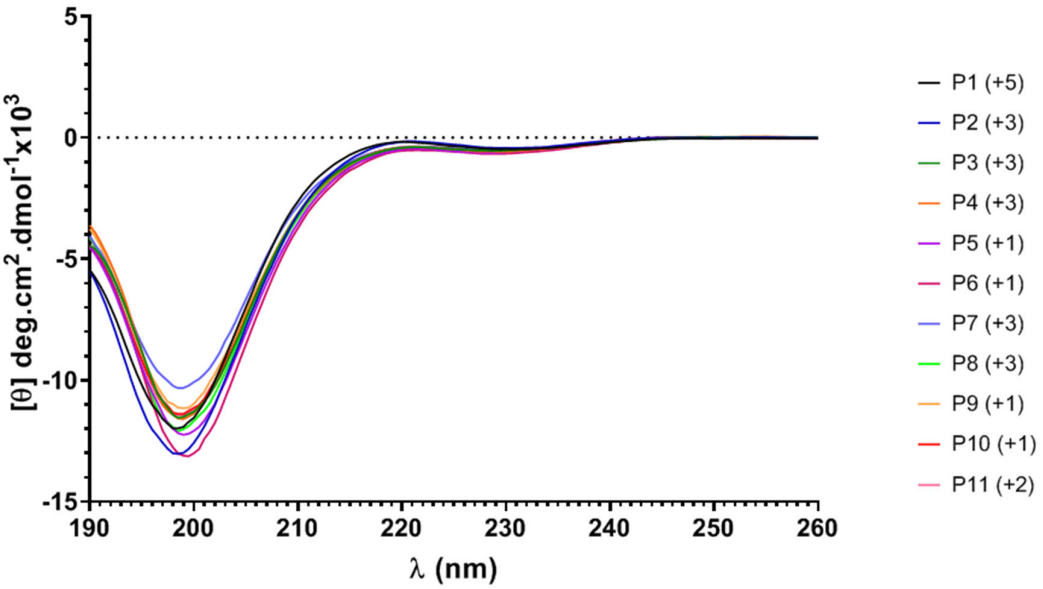


Figure S2. CD Spectra of P1-P11 peptides in water. In the legend are indicated the peptides net charge at neutral pH.

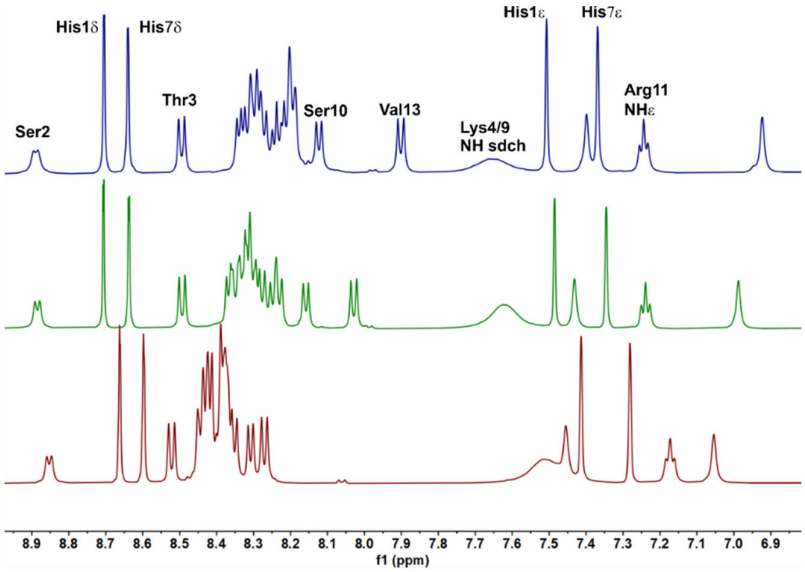


Figure S3. The aliphatic and amide regions of the P2 peptide ^{1}H NMR spectra in 90:10 H_2O/D_2O, 70:30 and 50:50 v:v H_2O/TFE-d2 (pH = 3, 500 MHz, 298 K) are shown in red, green and blue, respectively.

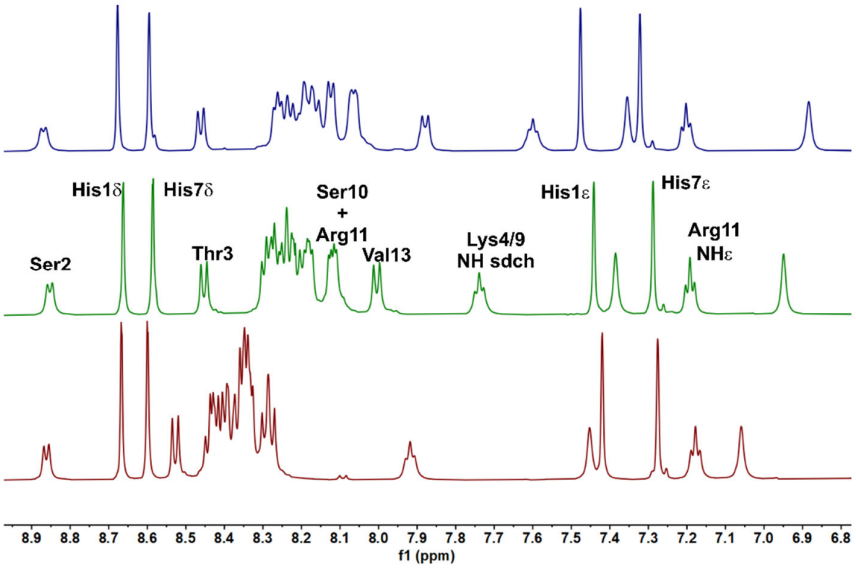


Figure S4. The aliphatic and amide regions of the P10 peptide ^{1}H NMR spectra in 90:10 H_2O/D_2O, 70:30 and 50:50 (v:v) H_2O/TFE-d_2 (pH = 3, 500 MHz, 298 K) are shown in red, green and blue, respectively.

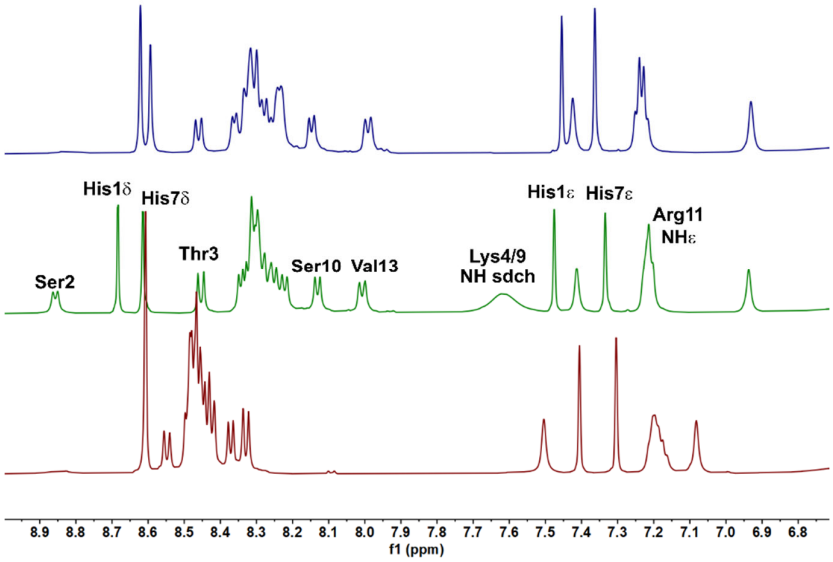


Figure S5. The aliphatic and amide regions of the P1 peptide ^{1}H NMR spectra in 90:10 H_2O/D_2O, 70:30 and 50:50 (v/v) H_2O/TFE-d_2 (pH = 3, 500 MHz, 298 K) are shown in red, green and blue, respectively.

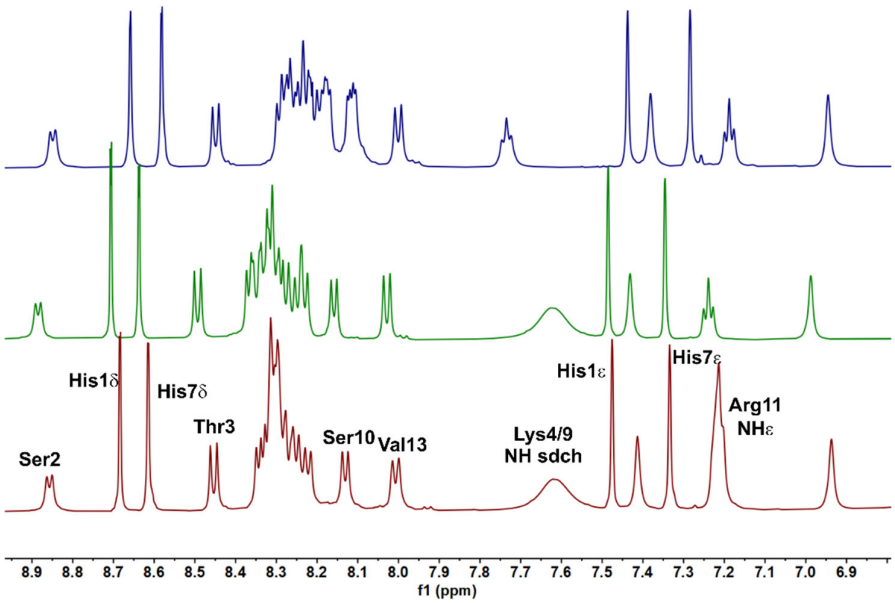
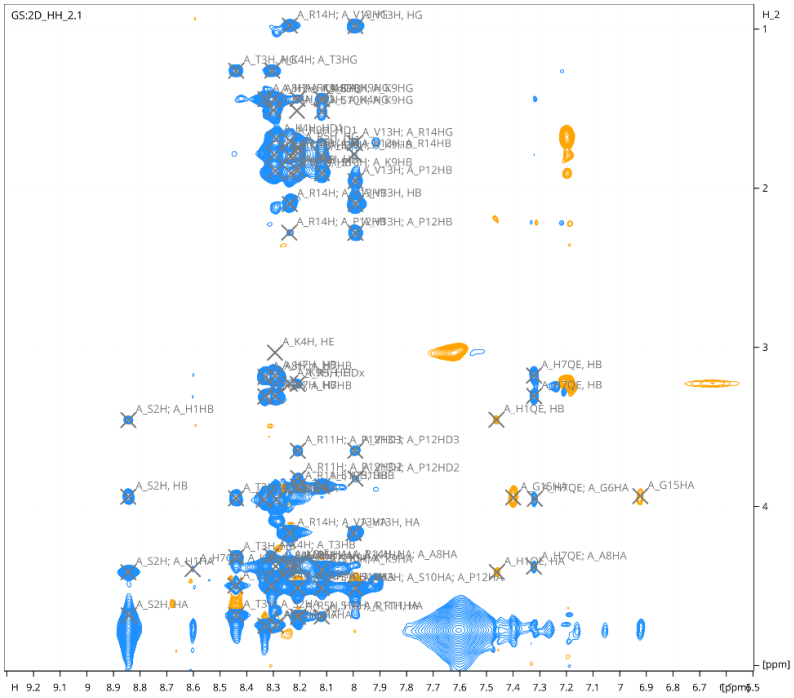


Figure S6. A comparison of the amide region of the ^{1}H NMR spectra of the P1 (red), P2 (green) and P10 (blue) peptides in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K).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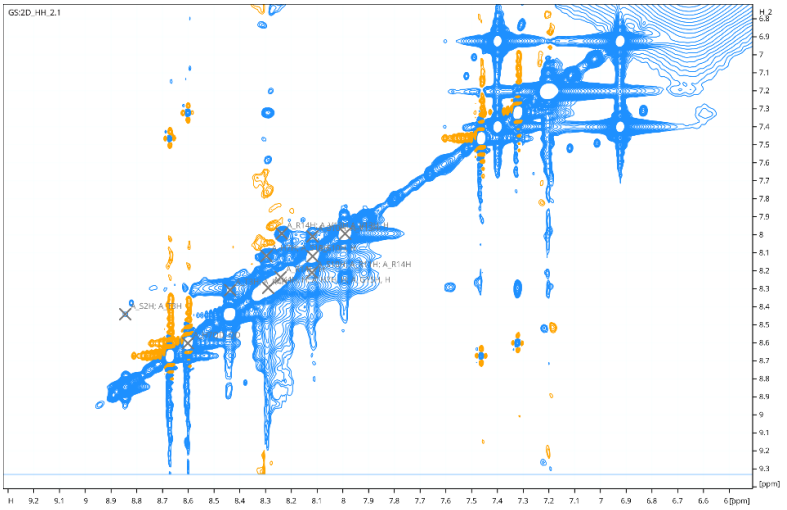
A_R14H; A_V13H, HG
A_T3H, HG; A_T3HG
A_K4H, HE
A_H7QE, HB
A_H1QE, HB
A_S2H; A_H1HB
A_R11H; A_P12HD3
A_R11H; A_P12HD2
A_S2H, HB
A_G15HA
A_R14H; A_V13H, HA
A_S2H; A_H1HA
A_H7QE; A_A8HA
A_S2H, HA
A_S10HA; A_P12HA
[ppm]


GS:2D_HH_2.1
[ppm]

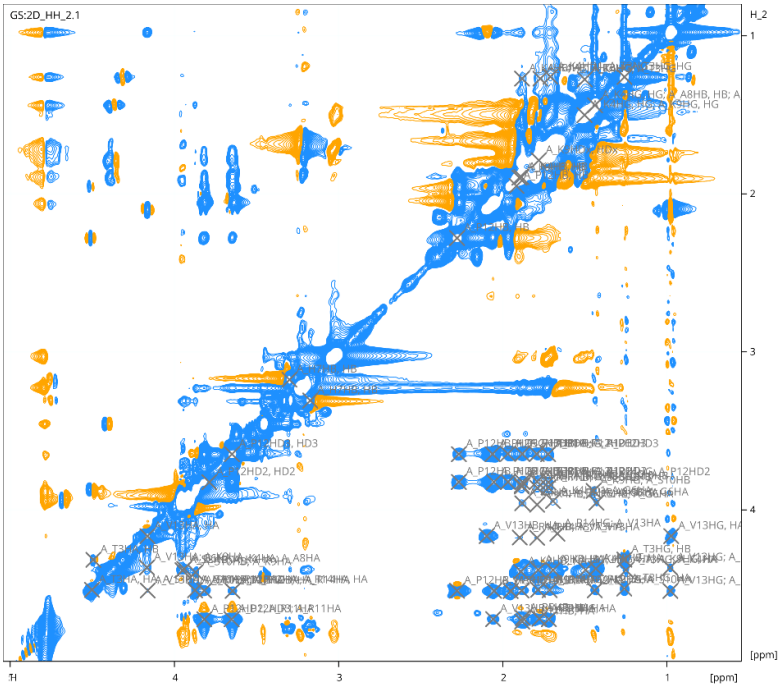
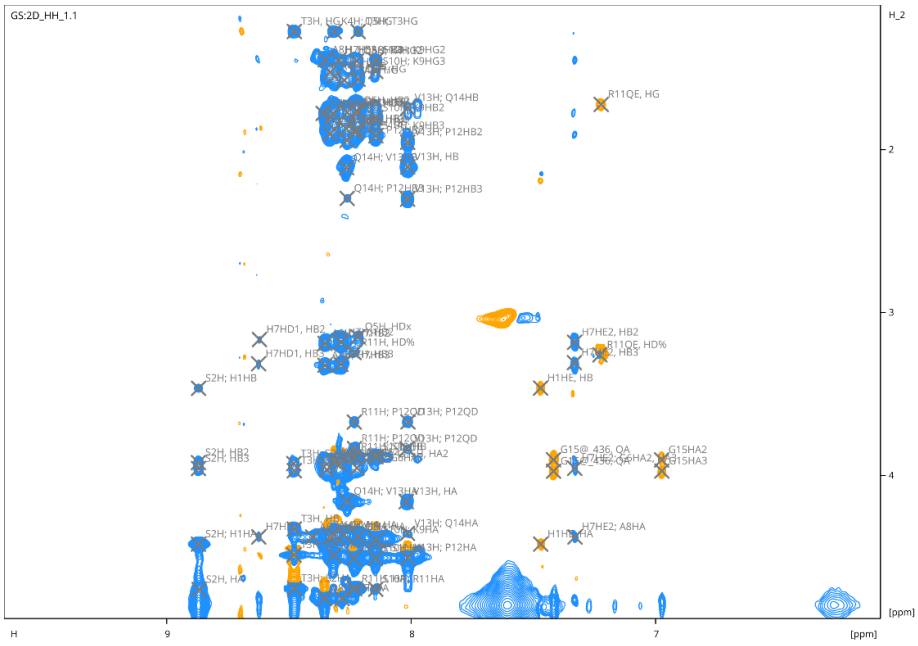


Figure S7. (Pages 19 and 20) Selected regions of the 2D NOESY spectrum of P1 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.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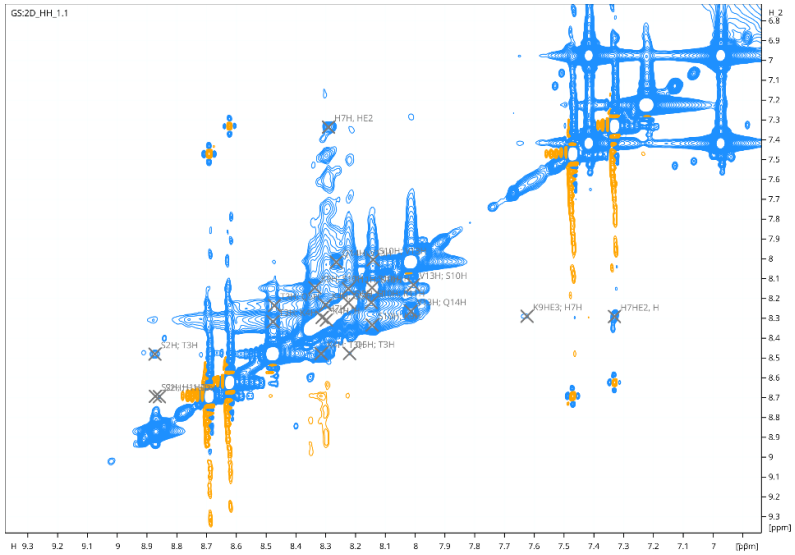
H_2
R11QE, HG
H7HD1, HB2
H7HD1, HB3
S2H; H1HB
H7HE2, HB2
R11QE, HD%
H1HE, HB
G15@ 436, QA
G15HA2
G15HA3
S2H, HB2
S2H, HB3
Q14H; V13H; V13H, HA
H7HE2; A8HA
S2H; H1HA
S2H, HA
2
3
4
H
9
8
7
[ppm]
[ppm]


GS:2D_HH_1.1
H_2
H7H, HE2
K9HE3; H7H
H7HE2, H
S2H; T3H
T3H; T3H
6.8
6.9
7
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8
8.1
8.2
8.3
8.4
8.5
8.6
8.7
8.8
8.9
9
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9.2
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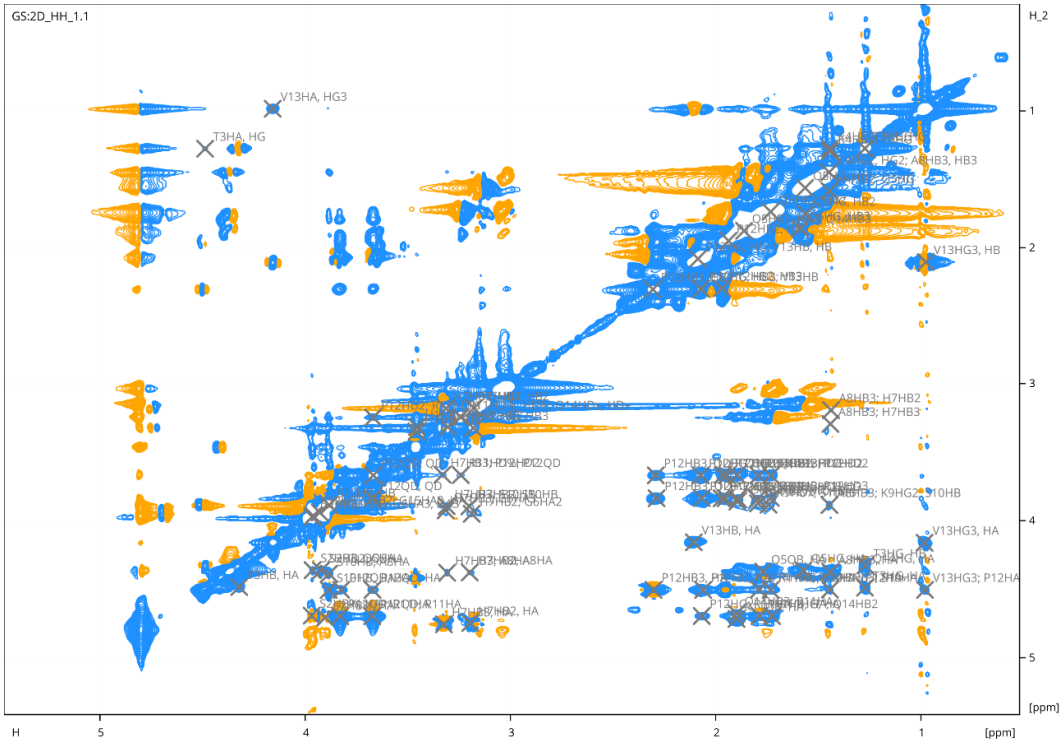

Figure S8. (Pages 21 and 22) Selected regions of the 2D NOESY spectrum of P2 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.


GS:2D_HH_2.1
H_2
Q14H; V13HG%
V13H, HG%
T3H, HG%
K9@_330, HGx
K9@_330, HG
K9@_330, HD1%
Q14H; V13HB%
V13H, HB%
Q14H; P12HB%
V13H; P12HB%
K9@_330, HE%
H7HB, HE
S2H; H1HB%
H1HE, HB%
S2H, HB%
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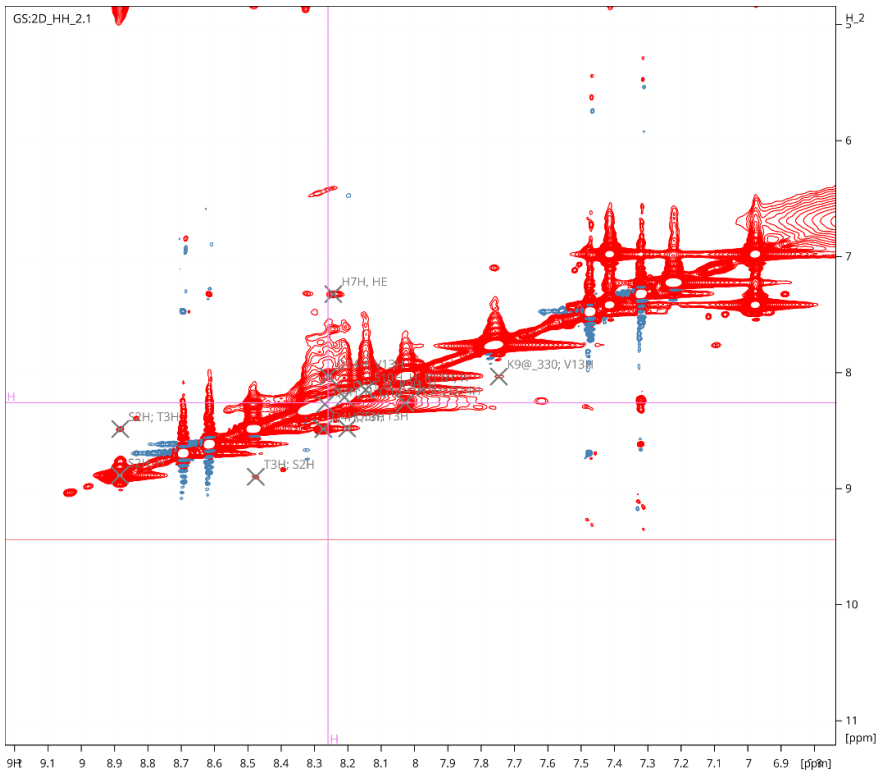
S2H, HA
H1HE, HA
[ppm]


GS:2D_HH_2.1
H_2
H7H, HE
K9@_330; V13H
S2H; T3H
T3H; S2H
[ppm]

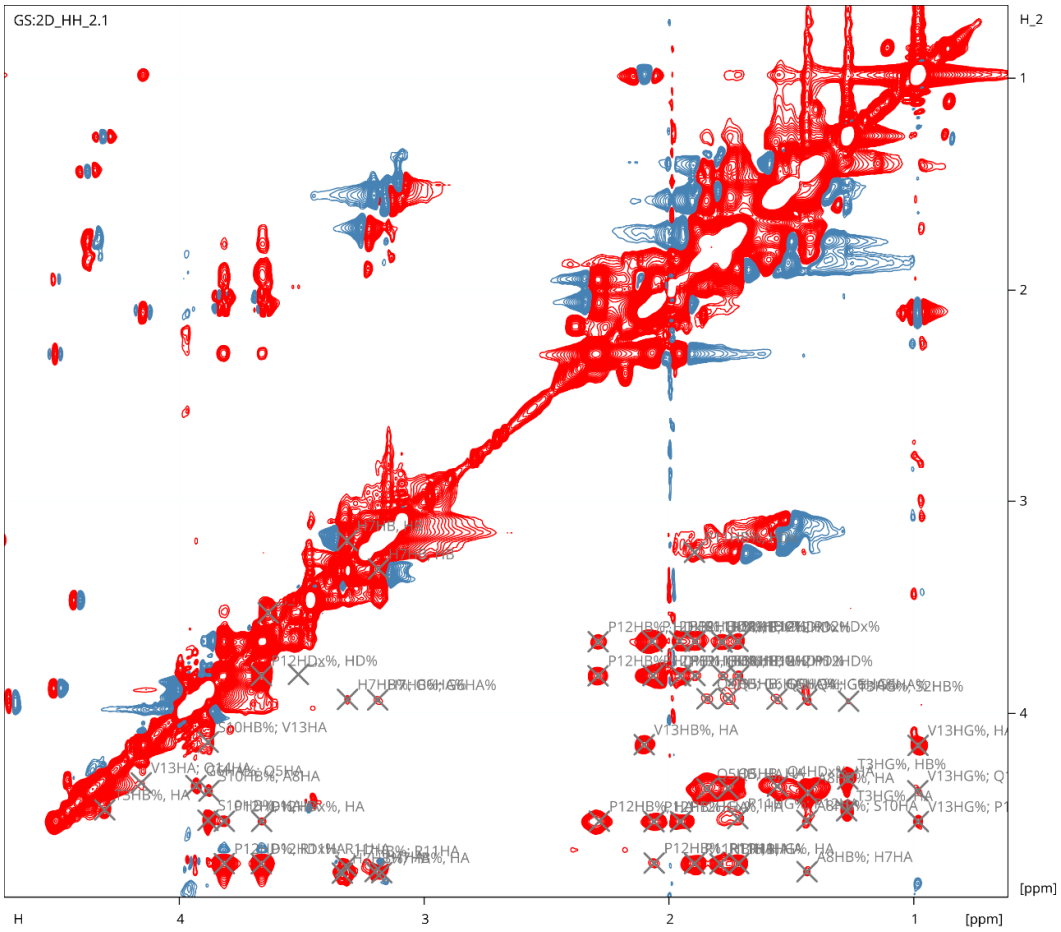


Figure S9. (Pages 23 and 24) Selected regions of the 2D NOESY spectrum of P10 peptide in a 70:30 (v/v) solution of H_2O/TFE-d2 at pH 3 (500 MHz, 298 K). The regions are displayed at different levels to make the lower-intensity correlation peaks more visible.

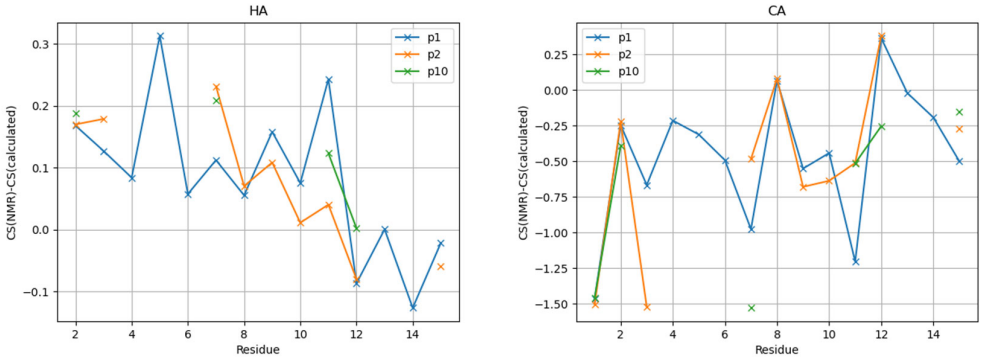


Figure S10. Chemical Shift (CS) difference between the experimental (NMR) and calculated CS from the peptide trajectories for the HA and the CA atoms. Sparta+ can only calculate the CS of residues without post-translational modifications, which is why some CS are missing.

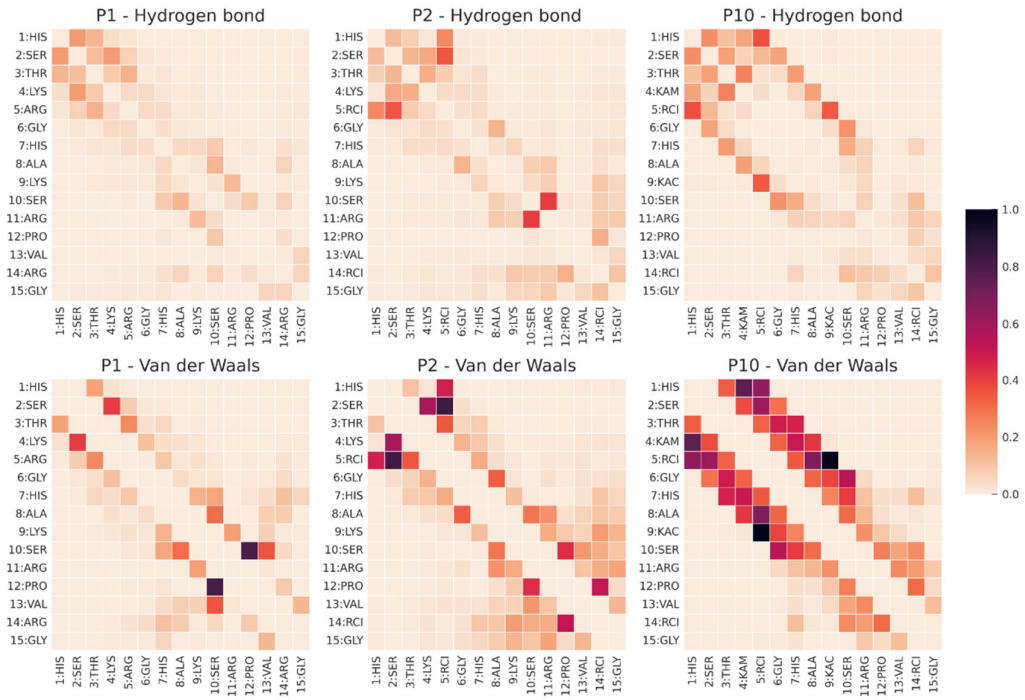


Figure S11. Intramolecular contacts arising from the Molecular Dynamics trajectories. The i,i+3 and i,i+4 contacts are typical of α-helices and more prevalent in P10. P2 shows more contacts than P1 because it is more compact, especially in the C-term region. This region is similar to P10 region, as expected because they share the same sequence.

Table S1. Peptides net charge and estimation of the α-helix content according to molar ellipticity at 222nm.

Peptide	Net charge (pH=7)	% α-helix
P1	**+5**	**9**
P2	**+3**	**19**
P3	**+3**	**18**
P4	**+3**	**22**
P5	**+1**	**24**
P6	**+1**	**21**
P7	**+3**	**14**
P8	**+3**	**20**
P9	**+1**	**16**
P10	**+1**	**23**
P11	**+2**	**18**

Table S2. P1 peptide NOE restraints in 30% TFE.

Assign F1	Assign F2	Pos F1	Pos F2	interval	classification
				Å	NOEs NMR
A.7.HIS.HB1	A.7.HIS.HB2	3.173	3.308		
A.7.HIS.HB2	A.7.HIS.HB1	3.308	3.173		
A.2.SER.H	A.1.HIS.HA	8.844	4.412	1.8-3.3	medium
A.2.SER.H	A.1.HIS.HB	8.844	3.456	> 5.5	very weak
A.3.THR.H	A.2.SER.HA	8.440	4.681	1.8-3.3	medium
A.2.SER.H	A.2.SER.HA	8.842	4.684	1.8-3.3	medium
A.3.THR.H	A.2.SER.HB	8.440	3.948	1.8-5.5	weak
A.2.SER.H	A.2.SER.HB	8.844	3.938	1.8-5.5	weak
A.2.SER.H	A.3.THR.H	8.845	8.441	1.8-5.5	weak
A.4.LYS.H	A.3.THR.HA	8.307	4.498	1.8-3.3	medium
A.3.THR.HG	A.3.THR.HA	1.260	4.498	1.8-5.5	weak
A.3.THR.HA	A.3.THR.HB	4.494	4.316	1.8-5.5	weak
A.3.THR.H	A.3.THR.HB	8.440	4.318	1.8-5.5	weak
A.3.THR.HG	A.3.THR.HB	1.259	4.315	1.8-3.3	medium
A.4.LYS.HB2	A.3.THR.HG	1.883	1.271	> 5.5	very weak
A.4.LYS.HD	A.3.THR.HG	1.710	1.259	> 5.5	very weak
A.3.THR.H	A.3.THR.HG	8.439	1.261	1.8-5.5	weak
A.4.LYS.H	A.3.THR.HG	8.304	1.261	1.8-5.5	weak
A.4.LYS.HG	A.3.THR.HG	1.501	1.276	1.8-5.5	weak
A.3.THR.H	A.4.LYS.H	8.438	8.307	1.8-3.3	medium
A.4.LYS.H	A.4.LYS.HA	8.291	4.376	1.8-2.5	strong
A.3.THR.HG	A.4.LYS.HA	1.250	4.382	> 5.5	very weak
A.2.SER.HB	A.4.LYS.HA	3.951	4.382	1.8-5.5	weak
A.4.LYS.H	A.4.LYS.HB2	8.293	1.890	1.8-5.5	weak
A.4.LYS.H	A.4.LYS.HB1	8.297	1.789	1.8-3.3	medium
A.4.LYS.H	A.4.LYS.HD	8.289	1.691	1.8-5.5	weak
A.4.LYS.H	A.4.LYS.HG	8.300	1.509	1.8-5.5	weak
A.5.ARG.HG	A.5.ARG.HA	1.719	4.692	1.8-5.5	weak
A.5.ARG.HB1	A.5.ARG.HA	1.777	4.690	1.8-3.3	medium
A.5.ARG.HB2	A.5.ARG.HA	1.878	4.685	1.8-5.5	weak
A.5.ARG.H	A.5.ARG.HB2	8.209	1.887	1.8-3.3	medium
A.5.ARG.H	A.5.ARG.HB1	8.209	1.780	1.8-3.3	medium
A.5.ARG.H	A.5.ARG.HD	8.208	3.229	1.8-5.5	weak
A.5.ARG.H	A.5.ARG.HG	8.208	1.743	1.8-5.5	weak
A.6.GLY.H	A.6.GLY.HA	8.288	3.955	1.8-3.3	medium
A.4.LYS.HD	A.6.GLY.HA	1.694	3.944	> 5.5	very weak
A.7.HIS.NHE	A.6.GLY.HA	7.318	3.951	1.8-5.5	weak
A.8.ALA.HB	A.6.GLY.HA	1.429	3.954	> 5.5	very weak
A.8.ALA.H	A.7.HIS.HA	8.330	4.749	1.8-3.3	medium
A.7.HIS.H	A.7.HIS.HA	8.290	4.746	1.8-3.3	medium
A.7.HIS.H	A.7.HIS.HB1	8.293	3.179	1.8-5.5	weak
A.7.HIS.HE	A.7.HIS.HB2	7.321	3.305	1.8-5.5	weak

A.7.HIS.HE	A.7.HIS.HB1	7.322	3.176	1.8-5.5	weak
A.7.HIS.H	A.8.ALA.HB	8.296	1.441	1.8-5.5	weak
A.8.ALA.H	A.7.HIS.HB2	8.330	3.308	1.8-5.5	weak
A.8.ALA.H	A.7.HIS.HB1	8.330	3.185	1.8-5.5	weak
A.7.HIS.H	A.7.HIS.HB2	8.293	3.304	1.8-5.5	weak
A.8.ALA.HB	A.8.ALA.HA	1.433	4.371	1.8-3.3	medium
A.7.HIS.HE	A.8.ALA.HA	7.322	4.378	1.8-5.5	weak
A.9.LYS.HB2	A.9.LYS.HA	1.889	4.391	1.8-3.3	medium
A.8.ALA.H	A.9.LYS.HG	8.330	1.439	1.8-5.5	weak
A.9.LYS.HB2	A.9.LYS.HA	1.784	4.380	1.8-3.3	medium
A.13.VAL.HA	A.9.LYS.HA	4.167	4.365	1.8-5.5	weak
A.10.SER.HB	A.9.LYS.HA	3.872	4.395	1.8-5.5	weak
A.10.SER.H	A.9.LYS.HA	8.117	4.399	1.8-2.5	strong
A.9.LYS.H	A.9.LYS.HB1	8.235	1.800	1.8-5.5	weak
A.9.LYS.H	A.9.LYS.HB2	8.232	1.906	1.8-5.5	weak
A.10.SER.H	A.9.LYS.HB2	8.117	1.905	1.8-5.5	weak
A.10.SER.H	A.9.LYS.HB1	8.118	1.796	1.8-5.5	weak
A.10.SER.H	A.9.LYS.HG2	8.117	1.515	1.8-5.5	weak
A.10.SER.H	A.9.LYS.HG1	8.117	1.440	1.8-5.5	weak
A.11.ARG.HB2	A.10.SER.HB	1.884	3.844	1.8-5.5	weak
A.11.ARG.HB1	A.10.SER.HB	1.789	3.861	1.8-5.5	weak
A.11.ARG.HG	A.10.SER.HB	1.721	3.858	> 5.5	very weak
A.11.ARG.H	A.9.LYS.HG1	8.209	1.437	> 5.5	very weak
A.11.ARG.H	A.9.LYS.HG2	8.212	1.513	> 5.5	very weak
A.10.SER.H	A.10.SER.HA	8.118	4.511	1.8-3.3	medium
A.13.VAL.HB	A.10.SER.HA	2.053	4.513	1.8-3.3	medium
A.11.ARG.H	A.10.SER.HA	8.208	4.511	1.8-2.5	strong
A.9.LYS.HG1	A.10.SER.HA	1.439	4.509	1.8-5.5	weak
A.9.LYS.HG1	A.10.SER.HB	1.447	3.880	> 5.5	very weak
A.10.SER.H	A.10.SER.HB	8.117	3.873	1.8-5.5	weak
A.11.ARG.H	A.10.SER.HB	8.208	3.873	1.8-5.5	weak
A.13.VAL.HB	A.11.ARG.HA	2.059	4.691	1.8-5.5	weak
A.12.PRO.HD2	A.11.ARG.HA	3.818	4.692	1.8-5.5	weak
A.12.PRO.HD1	A.11.ARG.HA	3.651	4.693	1.8-5.5	weak
A.11.ARG.HG	A.12.PRO.HA	1.714	4.508	1.8-5.5	weak
A.11.ARG.HB1	A.12.PRO.HA	1.785	4.506	1.8-5.5	weak
A.11.ARG.HB2	A.12.PRO.HA	1.885	4.511	1.8-5.5	weak
A.11.ARG.HB	A.11.ARG.HA	1.882	4.707	1.8-5.5	weak
A.10.SER.H	A.11.ARG.HA	8.119	4.691	1.8-5.5	weak
A.10.SER.HB	A.12.PRO.HA	3,874	4,509	1.8-5.5	weak
A.12.PRO.HB2	A.12.PRO.HA	2.278	4.512	1.8-3.3	medium
A.12.PRO.HD2	A.12.PRO.HA	3.819	4.511	1.8-5.5	weak
A.12.PRO.HD1	A.12.PRO.HA	3.646	4.513	1.8-5.5	weak
A.14.ARG.H	A.12.PRO.HB2	8.240	2.278	> 5.5	very weak
A.13.VAL.H	A.12.PRO.HB1	7.992	1.954	1.8-5.5	weak
A.13.VAL.H	A.12.PRO.HB2	7.992	2.280	1.8-5.5	weak

A.13.VAL.H	A.12.PRO.HD2	7.991	3.824	> 5.5	very weak
A.13.VAL.H	A.12.PRO.HD1	7.992	3.649	> 5.5	very weak
A.12.PRO.HB1	A.12.PRO.HD2	2.267	3.824	1.8-5.5	weak
A.12.PRO.HB1	A.12.PRO.HD2	1.968	3.823	1.8-5.5	weak
A.11.ARG.HG	A.12.PRO.HD1	1.723	3.647	> 5.5	very weak
A.11.ARG.HB1	A.12.PRO.HD2	1.791	3.822	> 5.5	very weak
A.11.ARG.HB2	A.12.PRO.HD2	1.880	3.823	> 5.5	very weak
A.11.ARG.HB2	A.12.PRO.HD2	1.881	3.646	> 5.5	very weak
A.11.ARG.HB1	A.12.PRO.HD2	1.793	3.647	1.8-5.5	weak
A.11.ARG.HG	A.12.PRO.HD1	1.723	3.647	> 5.5	very weak
A.12.PRO.HG	A.12.PRO.HD2	2.054	3.823	1.8-3.3	medium
A.12.PRO.HG	A.12.PRO.HD1	2.062	3.647	1.8-3.3	medium
A.12.PRO.HB1	A.12.PRO.HD1	1.969	3.645	1.8-3.3	medium
A.12.PRO.HB2	A.12.PRO.HD1	2.267	3.648	1.8-5.5	weak
A.11.ARG.H	A.12.PRO.HD1	8.208	3.649	> 5.5	very weak
A.11.ARG.H	A.12.PRO.HD2	8.208	3,820	1.8-5.5	weak
A.10.SER.H	A.13.VAL.H	8.118	8.009	1.8-5.5	weak
A.14.ARG.H	A.13.VAL.H	8.238	7.993	1.8-5.5	weak
A.13.VAL.HG	A.13.VAL.HA	0.974	4.166	1.8-5.5	weak
A.13.VAL.HB	A.13.VAL.HA	2.098	4.166	1.8-5.5	weak
A.13.VAL.H	A.13.VAL.HA	7.999	4.168	1.8-3.3	medium
A.14.ARG.HB1	A.13.VAL.HA	1.790	4.176	> 5.5	very weak
A.14.ARG.HB2	A.13.VAL.HA	1.897	4.175	1.8-5.5	weak
A.14.ARG.H	A.13.VAL.HA	8.237	4.166	1.8-3.3	medium
A.14.ARG.HG	A.13.VAL.HA	1.667	4.151	1.8-5.5	weak
A.13.VAL.H	A.13.VAL.HB	7.992	2.098	1.8-3.3	medium
A.14.ARG.H	A.13.VAL.HB	8.238	2.098	1.8-5.5	weak
A.13.VAL.H	A.13.VAL.HG	7.992	0.980	1.8-5.5	weak
A.14.ARG.H	A.13.VAL.HG	8.238	0.978	1.8-5.5	weak
A.13.VAL.H	A.14.ARG.HB1	7.996	1.786	> 5.5	very weak
A.13.VAL.H	A.14.ARG.HG	7.994	1.716	> 5.5	very weak
A.15.GLY.H	A.15.GLY.HA	8.336	3.957	1.8-3.3	medium
A.13.VAL.HG	A.14.ARG.HA	0.980	4.366	> 5.5	very weak

Table S3. P2 peptide NOE restraints in 30% TFE

Assign F1	Assign F2	Pos F1	Pos F2	interval	classification
				Å	NOEs NMR
P2.2.SER.H	P2.1.HIS.HA	8.870	4.421	1.8 - 5.5	weak
P2.1.HIS.HB2	P2.1.HIS.HB1	3.456	3.317	1.8-3.3	medium
P2.1.HIS.HB2	P2.1.HIS.HB1	3.458	3.350		
P2.2.SER.H	P2.1.HIS.HB2	8.870	3.465	> 5.5	very weak
P2.2.SER.H	P2.1.HIS.HD	8.872	8.693	1.8-5.5	weak
P2.2.SER.H	P2.1.HIS.HD	8.859	8.691		
P2.3.THR.H	P2.2.SER.HA	8.477	4.693	1.8-2.5	strong
P2.2.SER.H	P2.2.SER.HA	8.868	4.700	1.8-3.3	medium
P2.2.SER.H	P2.2.SER.HB1	8.871	3.921	1.8-5.5	weak
P2.2.SER.H	P2.2.SER.HB2	8.870	3.957	1.8-5.5	weak
P2.3.THR.H	P2.2.SER.HB1	8.480	3.927	1.8-5.5	weak
P2.3.THR.H	P2.2.SER.HB2	8.478	3.970	1.8-5.5	weak
P2.5.CIT.H	P2.3.THR.H	8.220	8.477	> 5.5	very weak
P2.2.SER.H	P2.3.THR.H	8.873	8.480	1.8-5.5	weak
P2.4.LYS.H	P2.3.THR.H	8.316	8.479	1.8-5.5	weak
P2.3.THR.HB	P2.3.THR.HA	4.321	4.484	1.8-5.5	weak
P2.3.THR.HG	P2.3.THR.HA	1.272	4.489	1.8-5.5	weak
P2.4.LYS.H	P2.3.THR.HA	8.316	4.488	1.8-3.3	medium
P2.3.THR.HG	P2.3.THR.HB	1.271	4.327	1.8-3.3	medium
P2.3.THR.H	P2.3.THR.HB	8.478	4.328	1.8-5.5	weak
P2.4.LYS.HG1	P2.3.THR.HG	1.444	1.274	1.8-5.5	weak
P2.4.LYS.HG1	P2.3.THR.HG	1.443	1.296		
P2.3.THR.HA	P2.3.THR.HG	4.488	1.276	1.8-5.5	weak
P2.5.CIT.H	P2.3.THR.HG	8.217	1.275	> 5.5	very weak
P2.4.LYS.H	P2.3.THR.HG	8.315	1.275	1.8-5.5	weak
P2.3.THR.H	P2.3.THR.HG	8.478	1.275	1.8-5.5	weak
P2.3.THR.H	P2.4.LYS.H	8.477	8.317	1.8-3.3	medium
P2.4.LYS.H	P2.4.LYS.HB1	8.315	1.875	1.8-5.5	weak
P2.4.LYS.H	P2.4.LYS.HB2	8.319	1.776	1.8-3.3	medium
P2.5.CIT.H	P2.4.LYS.HG1	8.223	1.455	1.8-5.5	weak
P2.4.LYS.H	P2.4.LYS.HG2	8.314	1.551	1.8-5.5	weak
P2.4.LYS.H	P2.5.CIT.H	8.301	8.233	1.8-2.5	strong
P2.3.THR.H	P2.5.CIT.H	8.472	8.236	1.8-3.3	medium
P2.5.CIT.HB1	P2.5.CIT.HA	1.768	4.372	1.8-3.3	medium
P2.5.CIT.H	P2.5.CIT.HA	8.216	4.375	1.8-2.5	strong
P2.2.SER.HB2	P2.5.CIT.HA	3.964	4.361	> 5.5	very weak
P2.2.SER.HB1	P2.5.CIT.HA	3.923	4.363	1.8-5.5	weak
P2.5.CIT.HG	P2.5.CIT.HB1	1.561	1.751	1.8-3.3	medium
P2.5.CIT.HG	P2.5.CIT.HB2	1.588	1.858	1.8-3.3	medium
P2.5.CIT.H	P2.5.CIT.HD	8.218	3.148	1.8-5.5	weak
P2.5.CIT.H	P2.5.CIT.HG	8.217	1.568	1.8-5.5	weak
P2.8.ALA.H	P2.6.GLY.HA1	8.345	3.930	1.8-3.3	medium

P2.8.ALA.H	P2.6.GLY.HA2	8.345	3.966	1.8-2.5	strong
P2.7.HIS.HB1	P2.6.GLY.HA	3.189	3.950	1.8-5.5	weak
P2.7.HIS.HB2	P2.6.GLY.HA	3.319	3.941	1.8-5.5	weak
P2.7.HIS.HB2	P2.10.SER.HB	3.311	3.894	> 5.5	very weak
P2.7.HIS.HB1	P2.10.SER.HB	3.200	3.896	> 5.5	very weak
P2.7.HIS.HE	P2.6.GLY.HA	7.331	3.956	> 5.5	very weak
P2.5.CIT.H	P2.6.GLY.HA	8.222	3.954	1.8-5.5	weak
P2.7.HIS.HE	P2.7.HIS.H	7.331	8.291	1.8-5.5	weak
P2.9.LYS.ENH3+	P2.7.HIS.H	7.624	8.290	1.8-5.5	weak
P2.8.ALA.H	P2.7.HIS.HA	8.353	4.754	1.8-3.3	medium
P2.7.HIS.H	P2.7.HIS.HA	8.282	4.755	1.8-3.3	medium
P2.7.HIS.HD	P2.7.HIS.HB1	8.621	3.165	> 5.5	very weak
P2.7.HIS.HE	P2.7.HIS.HB1	7.331	3.182	1.8-5.5	weak
P2.7.HIS.HD	P2.7.HIS.HB2	8.624	3.314	1.8-5.5	weak
P2.7.HIS.HE	P2.7.HIS.HB2	7.332	3.307	1.8-5.5	weak
P2.7.HIS.H	P2.7.HIS.HB1	8.287	3.182	1.8-5.5	weak
P2.7.HIS.H	P2.7.HIS.HB2	8.287	3.318	1.8-5.5	weak
P2.8.ALA.H	P2.7.HIS.HB1	8.353	3.189	1.8-5.5	weak
P2.8.ALA.H	P2.7.HIS.HB2	8.353	3.323	1.8-5.5	weak
P2.7.HIS.HB1	P2.7.HIS.HB2	3.181	3.323		
P2.7.HIS.HB2	P2.7.HIS.HB1	3.314	3.181		
P2.8.ALA.HB	P2.7.HIS.HB2	1.441	3.295	> 5.5	very weak
P2.8.ALA.HB	P2.7.HIS.HB1	1.437	3.195	> 5.5	very weak
P2.7.HIS.HE	P2.8.ALA.HA	7.330	4.377	1.8-5.5	weak
P2.7.HIS.HB1	P2.8.ALA.HA	3,199	4,378	> 5.5	very weak
P2.7.HIS.HB2	P2.8.ALA.HA	3.308	4.380	> 5.5	very weak
P2.9.LYS.H	P2.8.ALA.HA	8.334	4.377	1.8-2.5	strong
P2.8.ALA.HB	P2.8.ALA.HA	1.441	4.374	1.8-3.3	medium
P2.10.SER.HB	P2.8.ALA.HA	3.884	4.387	1.8-5.5	weak
P2.8.ALA.H	P2.8.ALA.HB	8.351	1.448	1.8-3.3	medium
P2.7.HIS.H	P2.8.ALA.HB	8.298	1.450	1.8-5.5	weak
P2.10.SER.H	P2.9.LYS.H	8.144	8.334	1.8-3.3	medium
P2.10.SER.H	P2.9.LYS.HA	8.144	4.395	1.8-2.5	strong
P2.10.SER.H	P2.9.LYS.HB1	8.145	1.805	1.8-5.5	weak
P2.10.SER.H	P2.9.LYS.HB2	8.145	1.915	1.8-5.5	weak
P2.9.LYS.H	P2.9.LYS.HB1	8.330	1.801	1.8-3.3	medium
P2.9.LYS.H	P2.9.LYS.HB2	8.331	1.905	1.8-5.5	weak
P2.10.SER.H	P2.9.LYS.HG1	8.144	1.450	1.8-5.5	weak
P2.10.SER.H	P2.9.LYS.HG2	8.145	1.507	1.8-5.5	weak
P2.9.LYS.H	P2.9.LYS.HG2	8.331	1.524	1.8-5.5	weak
P2.13.VAL.H	P2.10.SER.H	8,131	8,005	1.8-5.5	weak
P2.9.LYS.H	P2.10.SER.H	8.336	8.146	1.8-3.3	medium
P2.10.SER.H	P2.11.ARG.H	8.147	8.220	1.8-3.3	medium
P2.10.SER.H	P2.10.SER.HA	8.146	4.508	1.8-3.3	medium
P2.10.SER.HB	P2.10.SER.HA	3.886	4.506	1.8-3.3	medium
P2.8.ALA.HB	P2.10.SER.HA	1.443	4.503	1.8-5.5	weak

P2.11.ARG.H	P2.10.SER.HA	8.233	4.508	1.8-2.5	strong
P2.9.LYS.HD	P2.10.SER.HB	1.743	3.883	> 5.5	very weak
P2.10.SER.H	P2.10.SER.HB	8.144	3.885	1.8-5.5	weak
P2.11.ARG.H	P2.10.SER.HB	8.233	3.886	1.8-5.5	weak
P2.11.ARG.H	P2.11.ARG.HA	8.231	4.696	1.8-3.3	medium
P2.12.PRO.HD	P2.11.ARG.HA	3.674	4.697	1.8-5.5	weak
P2.12.PRO.HD	P2.11.ARG.HA	3.829	4.697	1.8-5.5	weak
P2.12.PRO.HG	P2.11.ARG.HA	2,068	4,695	1.8-5.5	weak
P2.11.ARG.HG	P2.11.ARG.HA	1.725	4.696	1.8-5.5	weak
P2.10.SER.H	P2.11.ARG.HA	8.145	4.698	1.8-5.5	weak
P2.14.CIT.HB2	P2.11.ARG.HA	1,898	4,677	1.8-5.5	weak
P2.11.ARG.HB2	P2.11.ARG.HA	1.899	4.717	1.8-5.5	weak
P2.11.ARG.H	P2.11.ARG.HD	8,234	3,245	> 5.5	very weak
P2.12.PRO.HD1	P2.12.PRO.HD2	3,673	3,836	1.8-2.5	strong
P2.12.PRO.HD1	P2.11.ARG.HD	3.669	3.248	> 5.5	very weak
P2.14.CIT.HB1	P2.12.PRO.HA	1.789	4.502	1.8-5.5	weak
P2.12.PRO.HG	P2.12.PRO.HA	2.061	4.505	1.8-5.5	weak
P2.12.PRO.HD2	P2.12.PRO.HA	3.825	4.505	1.8-5.5	weak
P2.12.PRO.HD1	P2.12.PRO.HA	3.672	4.505	1.8-5.5	weak
P2.13.VAL.H	P2.12.PRO.HA	8.015	4.505	1.8-2.5	strong
P2.14.CIT.H	P2.12.PRO.HB1	8.262	1.943	1.8-5.5	weak
P2.13.VAL.H	P2.12.PRO.HB1	8.014	1.954	1.8-5.5	weak
P2.13.VAL.H	P2.12.PRO.HB2	8.015	2.304	1.8-5.5	weak
P2.14.CIT.H	P2.12.PRO.HB2	8.262	2.299	> 5.5	very weak
P2.12.PRO.HB1	P2.12.PRO.HB2	1.969	2.296	1.8-2.5	strong
P2.12.PRO.HB1	P2.12.PRO.HD1	1.966	3.668	1.8-3.3	medium
P2.12.PRO.HB1	P2.12.PRO.HD1	1.944	3.669		
P2.12.PRO.HB1	P2.12.PRO.HD2	1.971	3.837	1.8-3.3	medium
P2.12.PRO.HB1	P2.12.PRO.HD2	1,952	3,837		
P2.14.CIT.HB1	P2.12.PRO.HD1	1.731	3.670	1.8-5.5	weak
P2.14.CIT.HB1	P2.12.PRO.HD1	1.792	3.670		
P2.14.CIT.HB1	P2.12.PRO.HD2	1.796	3.842	> 5.5	very weak
P2.14.CIT.HB1	P2.12.PRO.HD2	1.732	3.834		
P2.14.CIT.HB2	P2.12.PRO.HD2	1.894	3.838	> 5.5	very weak
P2.14.CIT.HB2	P2.12.PRO.HD1	1.896	3.668	1.8-5.5	weak
P2.11.ARG.H	P2.12.PRO.HD2	8.232	3.835	1.8-5.5	weak
P2.11.ARG.H	P2.12.PRO.HD1	8.233	3.672	1.8-5.5	weak
P2.13.VAL.H	P2.12.PRO.HD2	8.017	3.836	> 5.5	very weak
P2.13.VAL.H	P2.12.PRO.HD1	8.013	3.671	1.8-5.5	weak
P2.12.PRO.HB2	P2.12.PRO.HD2	2.288	3.837	1.8-3.3	medium
P2.12.PRO.HB2	P2.12.PRO.HD1	2.292	3.670	1.8-5.5	weak
P2.11.ARG.HD	P2.12.PRO.HD1	3.242	3.668	> 5.5	very weak
P2.12.PRO.HD1	P2.12.PRO.HD2	3.673	3.836	1.8-2.5	strong
P2.12.PRO.HG	P2.12.PRO.HD2	2.068	3.835	1.8-3.3	medium
P2.12.PRO.HG	P2.12.PRO.HD1	2.073	3.669	1.8-3.3	medium
P2.14.CIT.H	P2.13.VAL.H	8.265	8.017	1.8-3.3	medium

P2.13.VAL.H	**P2.13.VAL.HA**	**8.020**	**4.160**	**1.8-3.3**	**medium**
P2.13.VAL.HB	**P2.13.VAL.HA**	**2.106**	**4.158**	**1.8-3.3**	**medium**
P2.14.CIT.H	**P2.13.VAL.HA**	**8.263**	**4.159**	**1.8-2.5**	**strong**
P2.13.VAL.HG	**P2.13.VAL.HA**	**0.982**	**4.161**	**1.8-5.5**	**weak**
P2.14.CIT.H	**P2.13.VAL.HB**	**8.264**	**2.110**	**1.8-5.5**	**weak**
P2.13.VAL.H	**P2.13.VAL.HB**	**8.014**	**2.106**	**1.8-3.3**	**medium**
P2.13.VAL.HA	**P2.13.VAL.HG**	**4.158**	**0.984**	**1.8-5.5**	**weak**
P2.14.CIT.H	**P2.13.VAL.HG**	**8.264**	**0.985**	**> 5.5**	**very weak**
P2.13.VAL.H	**P2.13.VAL.HG**	**8.015**	**0.988**	**1.8-5.5**	**weak**
P2.13.VAL.H	**P2.14.CIT.H**	**8.014**	**8.264**	**1.8-3.3**	**medium**
P2.13.VAL.H	**P2.14.GLN.HA**	**8.015**	**4.355**	**1.8-5.5**	**weak**
P2.14.GLN.H	**P2.14.GLN.HA**	**8.274**	**4.365**	**1.8-3.3**	**medium**
P2.13.VAL.H	**P2.14.CIT.HB1**	**8.014**	**1.743**	**> 5.5**	**very weak**
P2.14.CIT.H	**P2.14.CIT.HB1**	**8.262**	**1.771**	**1.8-5.5**	**weak**
P2.14.CIT.H	**P2.14.CIT.HB2**	**8.265**	**1.872**	**1.8-5.5**	**weak**
P2.14.CIT.H	**P2.14.CIT.HG**	**8.274**	**1.574**	**1.8-5.5**	**weak**

Table S4. P10 peptide NOE restraints in 30% TFE

Assign F1	Assign F2	Pos F1	Pos F2	interval	classification
				Å	NOEs NMR
P10.7.HIS.HB1	P10.7.HIS.HB2	3.186	3.320		
P10.7.HIS.HB2	P10.7.HIS.HB1	3.315	3.186		
P10.2.SER.H	P10.1.HIS.HA	8.884	4.421	1.8-3.3	medium
P10.2.SER.H	P10.1.HIS.HB	8.885	3.468	> 5.5	very weak
P10.3.THR.H	P10.2.SER.H	8.476	8.897	1.8-5.5	weak
P10.3.THR.H	P10.2.SER.HA	8.482	4.692	1.8-3.3	medium
P10.2.SER.H	P10.2.SER.HA	8.883	4.702	1.8-5.5	weak
P10.3.THR.HG	P10.2.SER.HB	1.266	3.942	> 5.5	very weak
P10.2.SER.H	P10.2.SER.HB	8.885	3.943	1.8-5.5	weak
P10.3.THR.H	P10.2.SER.HB	8.481	3.947	1.8-5.5	weak
P10.4.hCIT.H	P10.3.THR.H	8.274	8.486	1.8-3.3	medium
P10.5.CIT.H	P10.3.THR.H	8.212	8.483	1.8-5.5	weak
P10.5.CIT.H	P10.3.THR.HA	8.210	4.451	1.8-3.3	medium
P10.4.hCIT.H	P10.3.THR.HA	8.274	4.459	1.8-3.3	medium
P10.3.THR.HG	P10.3.THR.HA	1.274	4.458	1.8-5.5	weak
P10.3.THR.HB	P10.3.THR.HA	4.305	4.454	1.8-5.5	weak
P10.3.THR.H	P10.3.THR.HA	8.482	4.459	1.8-3.3	medium
P10.3.THR.H	P10.3.THR.HB	8.484	4.312	1.8-3.3	medium
P10.3.THR.HG	P10.3.THR.HB	1.270	4.309	1.8-3.3	medium
P10.6.GLY.H	P10.3.THR.HG	8.319	1.277	1.8-5.5	weak
P10.4.hCIT.H	P10.3.THR.HG	8.275	1.275	1.8-5.5	weak
P10.5.CIT.H	P10.3.THR.HG	8.209	1.275	1.8-5.5	weak
P10.3.THR.H	P10.3.THR.HG	8.483	1.276	1.8-5.5	weak
P10.4.hCIT.HD	P10.4.hCIT.HA	1.557	4.343	1.8-5.5	weak
P10.4.hCIT.H	P10.4.hCIT.HB2	8.271	1.837	1.8-5.5	weak
P10.4.hCIT.H	P10.4.hCIT.HB1	8.269	1.754	1.8-3.3	medium
P10.4.hCIT.H	P10.4.hCIT.HG	8.276	1.423	1.8-5.5	weak
P10.5.CIT.HB1	P10.5.CIT.HA	1.758	4.353	1.8-3.3	medium
P10.5.CIT.HB2	P10.5.CIT.HA	1.845	4.355	1.8-3.3	medium
P10.6.GLY.H	P10.5.CIT.HA	8.307	4.340	1.8-2.5	strong
P10.6.GLY.HA	P10.5.CIT.HA	3.932	4.340	1.8-5.5	weak
P10.5.CIT.H	P10.5.GLN.HB2	8.209	1.853	1.8-3.3	medium
P10.5.CIT.H	P10.5.GLN.HB1	8.210	1.762	1.8-3.3	medium
P10.5.CIT.H	P10.5.CIT.HG	8.208	1.562	1.8-5.5	weak
P10.5.CIT.HG	P10.6.GLY.HA	1.559	3.932	1.8-5.5	weak
P10.5.CIT.HB1	P10.6.GLY.HA	1.758	3.930	1.8-5.5	weak
P10.5.CIT.HB2	P10.6.GLY.HA	1.845	3.931	1.8-5.5	weak
P10.7.HIS.HB1	P10.6.GLY.HA	3.190	3.936	1.8-5.5	weak
P10.7.HIS.HB2	P10.6.GLY.HA	3.313	3.934	1.8-5.5	weak
P10.6.GLY.H	P10.6.GLY.HA	8.308	3.934	1.8-2.5	strong
P10.7.HIS.H	P10.6.GLY.HA	8.242	3.935	1.8-2.5	strong
P10.4.hCIT.HG	P10.6.GLY.HA	1.437	3.933	1.8-5.5	weak

P10.7.HIS.HB1	P10.7.HIS.HA	3.173	4.750	1.8-3.3	medium
P10.8.ALA.HB	P10.7.HIS.HA	1.436	4.745	1.8-5.5	weak
P10.7.HIS.H	P10.7.HIS.HA	8.239	4.748	1.8-3.3	medium
P10.8.ALA.H	P10.7.HIS.HA	8.327	4.746	1.8-3.3	medium
P10.7.HIS.H	P10.7.HIS.HB2	8.240	3.324	1.8-5.5	weak
P10.7.HIS.H	P10.7.HIS.HB1	8.241	3.182	1.8-5.5	weak
P10.7.HIS.HD	P10.6.GLY.HA	8,616	3,935	> 5.5	very weak
P10.8.ALA.H	P10.7.HIS.HB2	8.326	3.327	1.8-5.5	weak
P10.8.ALA.H	P10.7.HIS.HB1	8.326	3.188	1.8-5.5	weak
P10.7.HIS.HE	P10.7.HIS.HB1	7.321	3.182	1.8-5.5	weak
P10.7.HIS.HE	P10.7.HIS.HB2	7.321	3.325	1.8-5.5	weak
P10.7.HIS.H	P10.7.HIS.HE	8.244	7.323	1.8-5.5	weak
P10.8.ALA.H	P10.8.ALA.HA	8.320	4.355	1.8-2.5	strong
P10.8.ALA.HB	P10.8.ALA.HA	1.433	4.373	1.8-3.3	medium
P10.10.SER.HB	P10.8.ALA.HA	3.879	4.365	1.8-5.5	weak
P10.8.ALA.H	P10.8.ALA.HB	8.327	1.439	1.8-3.3	medium
P10.8.ALA.HB	P10.10.SER.HA	1.437	4.505	1.8-5.5	weak
P10.10.SER.H	P10.8.ALA.HA	8.151	4.366	1.8-2.5	strong
P10.9.LYS.H	P10.9.LYS.HB2	8.306	1.849	1.8-5.5	weak
P10.9.LYS.H	P10.9.LYS.HB1	8.303	1.749	1.8-5.5	weak
P10.10.SER.H	P10.9.LYS.HG	8.149	1.551	1.8-5.5	weak
P10.9.LYS.H	P10.9.LYS.HG	8.310	1.569	1.8-5.5	weak
P10.10.SER.H	P10.9.LYS.HG	8.149	1.436	1.8-5.5	weak
P10.5.CIT.H	P10.9.LYS.HG	8.214	1.438	1.8-5.5	weak
P10.13.VAL.H	P10.14.CIT.H	8.029	8.261	1.8-3.3	medium
P10.10.SER.H	P10.10.SER.HA	8.145	4.506	1.8-2.5	strong
P10.10.SER.HB	P10.10.SER.HA	3.883	4.503	1.8-3.3	medium
P10.10.SER.H	P10.10.SER.HB	8.147	3.882	1.8-3.3	medium
P10.11.ARG.H	P10.11.ARG.HA	8.143	4.708	1.8-3.3	medium
P10.12.PRO.HD1	P10.11.ARG.HA	3.665	4.708	1.8-5.5	weak
P10.12.PRO.HD2	P10.11.ARG.HA	3.816	4.707	1.8-5.5	weak
P10.7.HIS.HB	P10.11.ARG.HA	3.320	4.718	1.8-5.5	weak
P10.11.ARG.HG	P10.11.ARG.HA	1.715	4.707	1.8-5.5	weak
P10.11.ARG.HB1	P10.11.ARG.HA	1.792	4.709	1.8-5.5	weak
P10.11.ARG.HB2	P10.11.ARG.HA	1.895	4.707	1.8-3.3	medium
P10.12.PRO.HB1	P10.11.ARG.HA	2.060	4.705	1.8-5.5	weak
P10.13.VAL.H	P10.11.ARG.HB1	8.029	1.774	1.8-5.5	weak
P10.13.VAL.H	P10.11.ARG.HG	8.029	1.729	1.8-5.5	weak
P10.11.ARG.H	P10.11.ARG.HB2	8.146	1.887	1.8-5.5	weak
P10.11.ARG.H	P10.11.ARG.HB1	8.145	1.775	1.8-3.3	medium
P10.11.ARG.H	P10.11.ARG.HD	8.144	3.227	1.8-5.5	weak
P10.11.ARG.HB2	P10.11.ARG.HD	1.896	3.241	1.8-5.5	weak
P10.11.ARG.H	P10.11.ARG.HG	8.144	1,725	1.8-5.5	weak
P10.13.VAL.H	P10.12.PRO.HA	8.029	4.510	1.8-2.5	strong
P10.12.PRO.HB2	P10.12.PRO.HA	2.285	4.508	1.8-2.5	strong
P10.12.PRO.HB1	P10.12.PRO.HA	2.061	4.510	1.8-3.3	medium

P10.12.PRO.HG	P10.12.PRO.HA	1.953	4.509	1.8-3.3	medium
P10.12.PRO.HD2	P10.12.PRO.HA	3.816	4.508	1.8-5.5	weak
P10.12.PRO.HD1	P10.12.PRO.HA	3.664	4.508	1.8-5.5	weak
P10.11.ARG.HG	P10.12.PRO.HA	1.719	4.495	1.8-5.5	weak
P10.13.VAL.HG	P10.12.PRO.HA	0.982	4.509	1.8-5.5	weak
P10.13.VAL.HG	P10.14.CIT.HA	0.984	4.364	1.8-5.5	weak
P10.13.VAL.H	P10.12.PRO.HB1	8.029	1.948	1.8-5.5	weak
P10.13.VAL.H	P10.12.PRO.HB2	8.030	2.301	1.8-5.5	weak
P10.14.CIT.H	P10.12.PRO.HB2	8.261	2.298	> 5.5	very weak
P10.14.CIT.H	P10.12.PRO.HB1	8.260	1.942	1.8-5.5	weak
P10.12.PRO.HB1	P10.12.PRO.HD2	2.065	3.822	1.8-3.3	medium
P10.12.PRO.HB1	P10.12.PRO.HD1	2.069	3.661	1.8-3.3	medium
P10.11.ARG.HB	P10.12.PRO.HD2	1.893	3.822	1.8-5.5	weak
P10.11.ARG.HB	P10.12.PRO.HD2	1.779	3.822	1.8-5.5	weak
P10.11.ARG.HB	P10.12.PRO.HD1	1.783	3.664	1.8-5.5	weak
P10.11.ARG.HB	P10.12.PRO.HD1	1.893	3.661	1.8-5.5	weak
P10.12.PRO.HB2	P10.12.PRO.HD2	2.290	3.823	1.8-5.5	weak
P10.12.PRO.HB2	P10.12.PRO.HD1	2.289	3.662	1.8-5.5	weak
P10.11.ARG.HG	P10.12.PRO.HD2	1.716	3.823	1.8-5.5	weak
P10.11.ARG.HG	P10.12.PRO.HD1	1.718	3.660	1.8-5.5	weak
P10.12.PRO.HD1	P10.12.PRO.HD2	3.665	3.822	1.8-2.5	strong
P10.13.VAL.H	P10.12.PRO.HD2	8.032	3.822	> 5.5	very weak
P10.13.VAL.H	P10.12.PRO.HD1	8.028	3.661	1.8-5.5	weak
P10.11.ARG.H	P10.12.PRO.HD2	8.144	3.821	1.8-5.5	weak
P10.11.ARG.H	P10.12.PRO.HD1	8.145	3.661	1.8-5.5	weak
P10.12.PRO.HG	P10.12.PRO.HD1	1.957	3.659	1.8-3.3	medium
P10.12.PRO.HG	P10.12.PRO.HD2	1.953	3.823	1.8-3.3	medium
P10.9.LYS.ENH	P10.13.VAL.H	7.747	8.034	1.8-5.5	weak
P10.14.GLN.H	P10.13.VAL.H	8.259	8.033	1.8-3.3	medium
P10.10.SER.HB	P10.13.VAL.HA	3.882	4.135	1.8-5.5	weak
P10.13.VAL.HB	P10.13.VAL.HA	2.101	4.147	1.8-3.3	medium
P10.13.VAL.H	P10.13.VAL.HA	8.032	4.152	1.8-3.3	medium
P10.14.CIT.H	P10.13.VAL.HA	8.260	4.150	1.8-2.5	strong
P10.13.VAL.HG	P10.13.VAL.HA	0.983	4.150	1.8-5.5	weak
P10.13.VAL.H	P10.13.VAL.HB	8.029	2.102	1.8-3.3	medium
P10.14.CIT.H	P10.13.VAL.HB	8.259	2.104	1.8-5.5	weak
P10.14.CIT.H	P10.13.VAL.HG	8.260	0.984	1.8-5.5	weak
P10.13.VAL.H	P10.13.VAL.HG	8.030	0.988	1.8-5.5	weak
P10.13.VAL.HA	P10.14.CIT.HA	4.155	4.327	1.8-5.5	weak
P10.13.VAL.H	P10.14.CIT.HA	8.033	4.363	1.8-5.5	weak
P10.13.VAL.HG	P10.14.CIT.HA	0.984	4.364	> 5.5	very weak