Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Controlling the conformational stability of coiled-coil peptides by a single stereogenic center of peripheral β-amino acid residue

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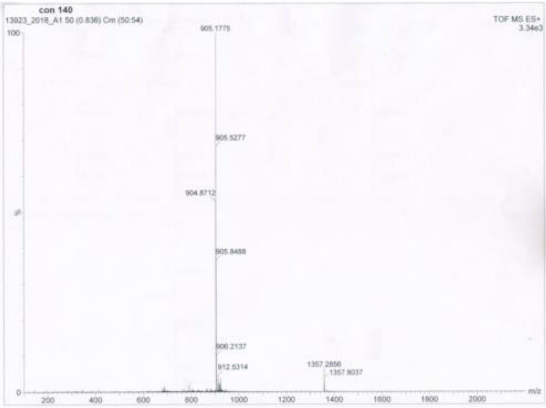
Table S1. The peptides analytical data.

Name	Formula	Calculated M/z	Experimental M/z	Analytical HPLC t_r [min]
1	$C_{125}H_{202}N_{32}O_{35}$	[(M+2H)/2] 1357.2598 [(M+3H)/3] 905.1758	[(M+2H)/2] 1357.2856 [(M+3H)/3] 905.1775	10.670
2	$C_{129}H_{208}N_{32}O_{35}$	[(M+2H)/2] 1384.2833 [(M+3H)/3] 923.1915	[(M+2H)/2] 1384.2961 [(M+3H)/3] 922.1913	10.597
3	$C_{126}H_{203}N_{31}O_{34}$	[(M+2H)/2] 1348.7648 [(M+3H)/3] 899.5125	[(M+2H)/2] 1348.7795 [(M+3H)/3] 899.5142	10.789
4	$C_{133}H_{214}N_{32}O_{35}$	[(M+3H)/3] 941.2072 [(M+4H)/4] 706.1573	[(M+3H)/3] 941.1786 [(M+4H)/4] 706.1364	11.355
5	$C_{129}H_{208}N_{32}O_{35}$	[(M+2H)/2] 1384.2833 [(M+3H)/3] 923.1915	[(M+2H)/2] 1384.9368 [(M+3H)/3] 923.5677	10.888
6	$C_{126}H_{203}N_{31}O_{34}$	[(M+2H)/2] 1348.7648 [(M+3H)/3] 899.5125	[(M+2H)/2] 1348.7467 [(M+3H)/3] 899.5209	10.867
7	$C_{133}H_{214}N_{32}O_{35}$	[(M+2H)/2] 1411.3068 [(M+3H)/3] 941.2072	[(M+2H)/2] 1411.3813 [(M+3H)/3] 941.2084	11.120

1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13923_2018_A1 50 (0.836) Cm (50:54)
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906.2137
912.5314
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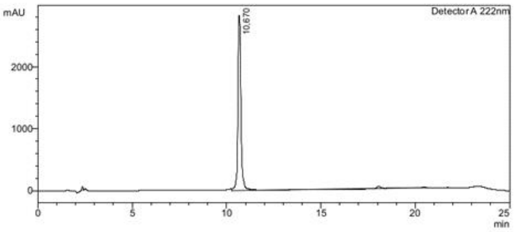
1357.8037
m/z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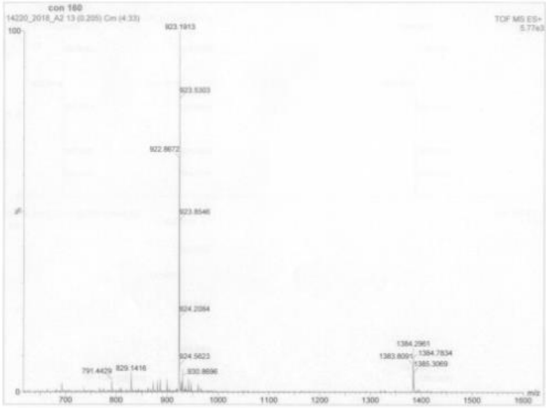
min

2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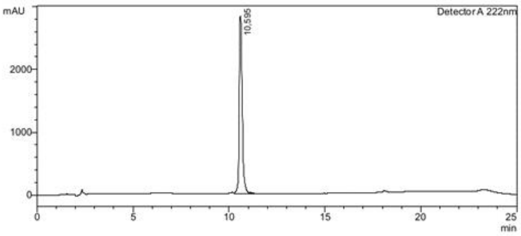
m/z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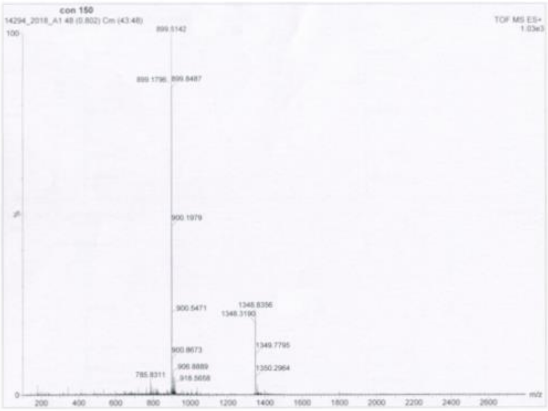
3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899.8487
900.1979
900.5471
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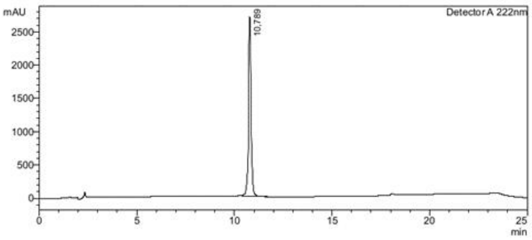
1348.3190
1349.7795
1350.2964
m/z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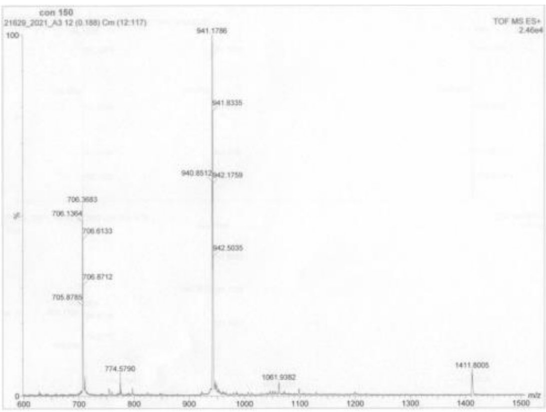
Detector A 222nm
10.789
min

4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21629_2021_A3 12 (0.188) Cm (12:117)
TOF MS ES+
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942.1759
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706.6133
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705.8785
774.5790
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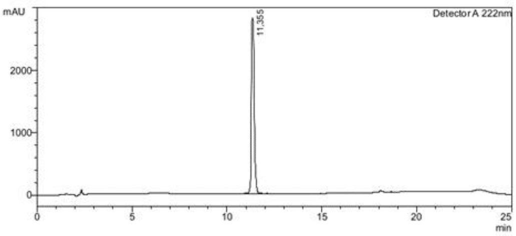
1411.8005
m/z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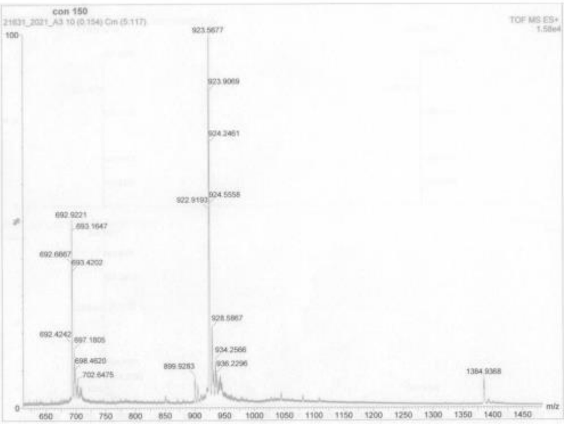
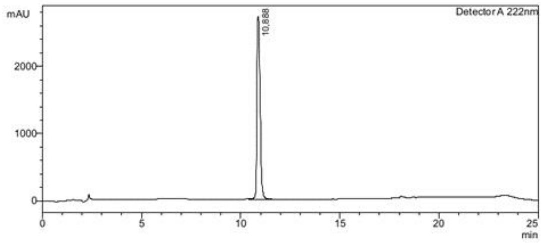
Detector A 222nm
11.355
min

5





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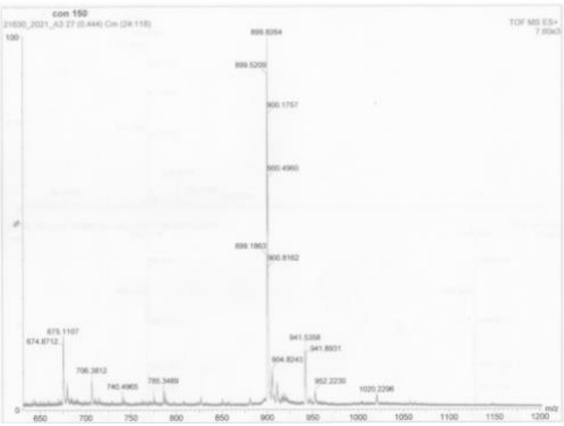

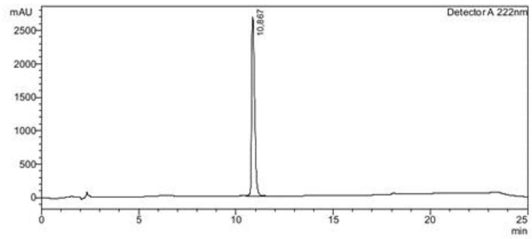

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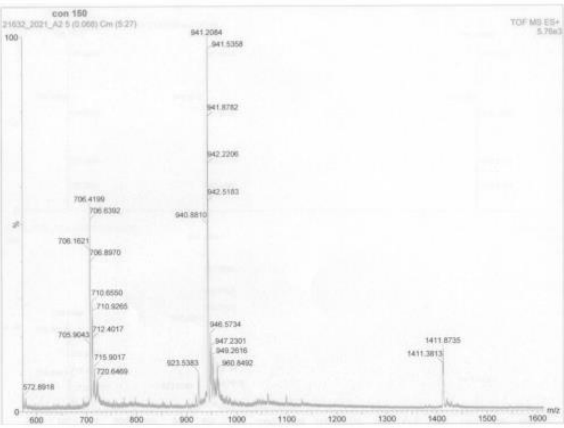


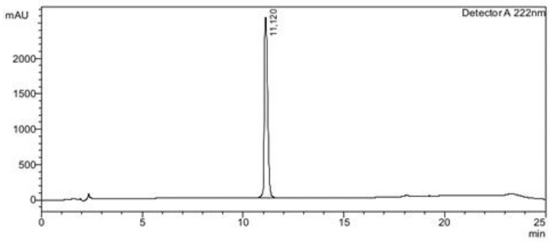


Fig. S1. MS spectra and the analytical HPLC chromatograms of the peptides **1**-**7**.

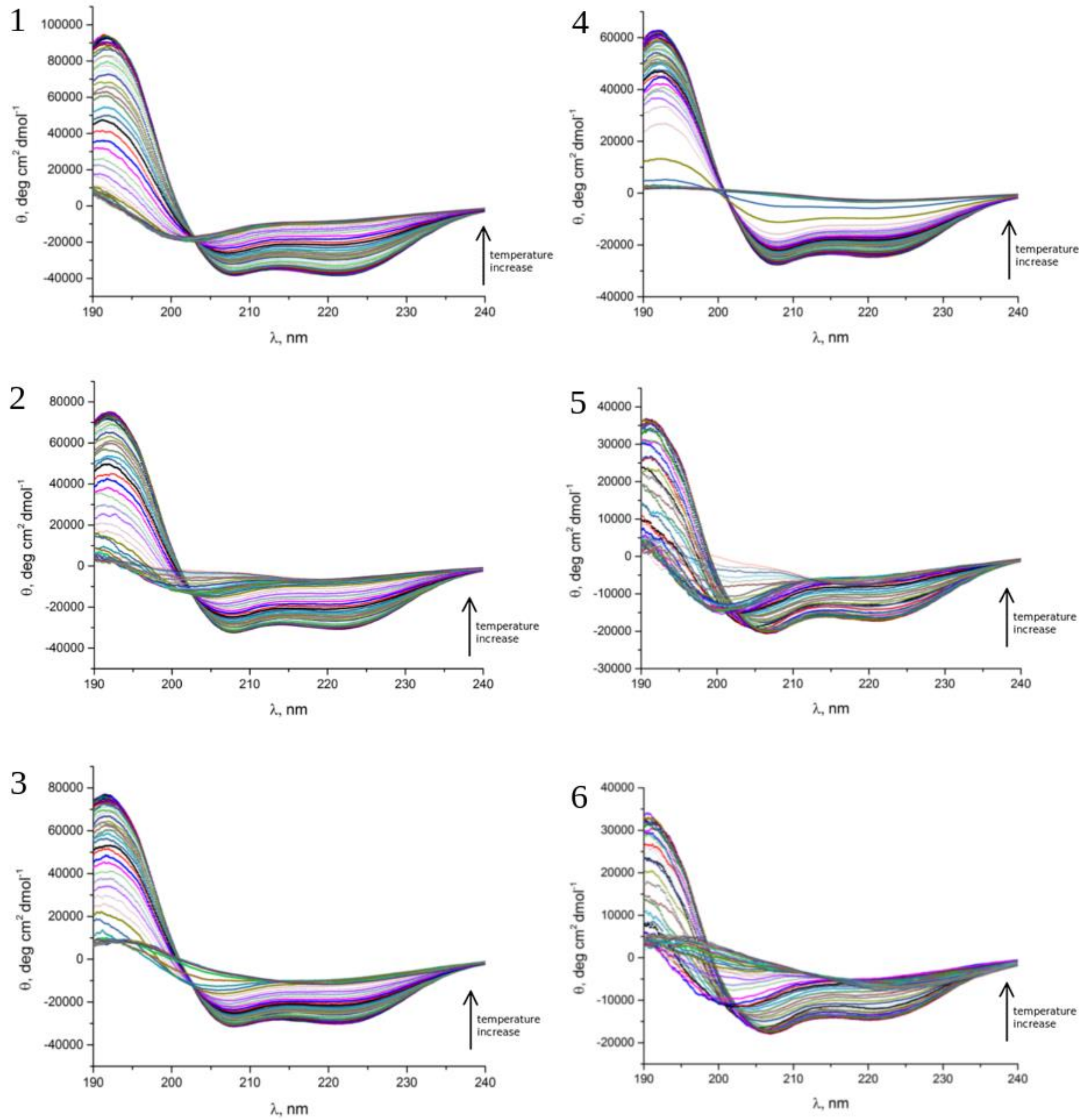


Fig. S2. CD spectra recorded in temperature range 4 – 98 ºC. $C_{pep.}$ = 80 μM; C_{buffer}=0.05 M; pH=7 for the peptides **1**-**6**.

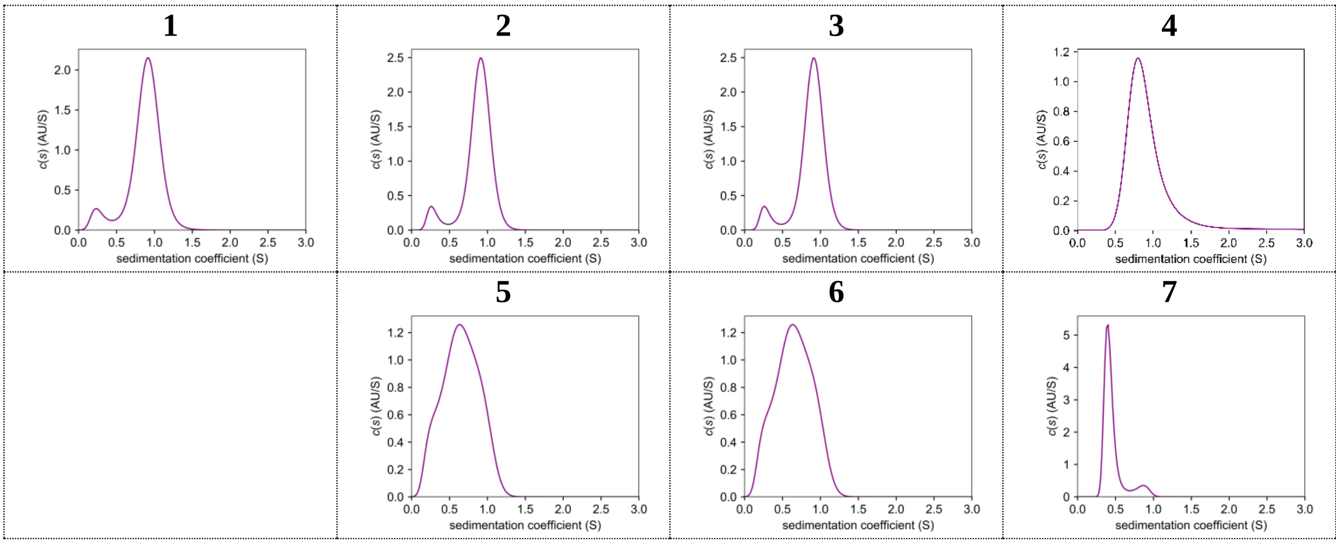


Fig. S3. Sedimentation coefficient distributions (c(s)) of the peptides **1-7** obtained using sedimentation velocity analytical ultracentrifugation (SV AUC).

Table S2. NMR assignments for peptide **2**.

Residue	Proton	Chemical shift [ppm]
Ac1	HA	1.93
Cp2	HN	8.12
	HA	2.59
	HB	4.22
	HG,D,E	1.55(3) 1.68(2) 2.01(1)
Glu3	HN	8.51
	HA	4.10
	HB	2.38
	HG	1.94(2) 2.00(1)
Ile4	HN	8.01
	HA	3.70
	HB	2.11
	HG1	1.21(2) 1.52(1)
	HG2	0.78
	HD	0.73
Ala5	HN	8.05
	HA	3.96
	HB	1.41
Ala6	HN	7.67
	HA	4.12
	HB	1.45
Ile7	HN	8.05
	HA	3.66
	HB	2.01
	HG1	0.96
	HG2	0.82
	HD	0.77
Lys8	HN	8.51
	HA	3.77
	HB	1.70(2) 1.83(1)
	HG	1.29
	HD	1.61
	HE	2.85
	NH_3Z	7.48
Gln9	HN	7.90
	HA	4.09
	HB	2.17
	HG	2.36(2) 2.46(1)
	HN'	6.75(2) 7.33(1)
Glu10	HN	8.06
	HA	4.14
	HB	2.00(2) 2.38(1)
	HG	2.37(2) 2.60(1)
Ile11	HN	8.49
	HA	3.51
	HB	1.90
	HG1	0.89
	HG2	0.78
	HD	0.73
Ala12	HN	7.78
	HA	3.95
	HB	1.42
Ala13	HN	7.69
	HA	4.18
	HB	1.49
Ile14	HN	8.18
	HA	3.66
	HB	1.97
	HG1	0.92
	HG2	0.83
	HD	0.77
Lys15	HN	8.51
	HA	3.76
	HB	1.66(2) 1.83(1)
	HG	1.28
	HD	1.56
	HE	2.81
	NH_3Z	7.48
Trp16	HN	7.92
	HA	4.35
	HB	3.33(2) 3.46(1)
	HD1	7.20
	HE3	7.53
	HZ3	7.04
	HZ2	7.40
	HH2	7.14
	HE1	10.02
Glu17	HN	8.18
	HA	3.94
	HB	2.38(2) 2.50(1)
	HG	2.41(2) 2.63(1)
Ile18	HN	8.51
	HA	3.52
	HB	1.78
	HG1	0.88(2) 0.97(1)
	HG2	0.77
	HD	0.73
Ala19	HN	7.58
	HA	3.94
	HB	1.34
Ala20	HN	7.48
	HA	3.92
	HB	1.15
Ile21	HN	7.79
	HA	3.70
	HB	1.87
	HG1	0.98
	HG2	0.77
	HD	0.73
Lys22	HN	8.08
	HA	3.92
	HB	1.71(2) 1.79(1)
	HG	1.31
	HD	1.55(2) 1.59(1)
	HE	2.85
	NH_3Z	7.48
Gln23	HN	7.84
	HA	4.10
	HB	1.98
	HG	2.31
	HN'	6.72(2) 7.33(1)
Gly24	HN	7.84
	HA	3.75(2) 3.81(1)
Tyr25	HN	7.83
	HA	4.46
	HB	2.84(2) 2.94(1)
	HD	6.98
	HE	6.67
Gly26	HN	8.14
	HA	3.72(2) 3.77(1)
NH_2	HN1	7.11
	HN2	6.99

H(i)-H(i+1)	**Intensity**
Ac1HA-Cp2HN	S
Cp2HA-Glu3HN	vS
Cp2CH$_2$1-Glu3HA	M
Glu3HA-Ile4HN	S
Glu3HB1-Ile4HN	S
Glu3HB2-Ile4HN	S
Glu3HG-Ile4HN	M
Glu3HN-Ile4HD	S
Ile4HA-Ala5HN	S
Ile4HB-Ala5HN	S
Ile4HG1(2)-Ala5HN	W
Ala5HA-Ala6HN	M
Ala5HB-Ala6HN	S
Ala5HN-Ala6HB	S
Ala6HA-Ile7HN	S
Ala6HN-Ile7HA	vW
Ala6HN-Ile7HB	W
Ile7HA-Lys8HN	M
Ile7HG2-Lys8HA	M
Ile7HD-Lys8HA	M
Ile7HD-Lys8HE	S
Ile7HN-Lys8HB1	M
Lys8HA-Gln9HN	M
Lys8HB1-Gln9HN	S
Lys8HB2-Gln9HN	W
Lys8HN-Gln9HB	vW
Gln9HA-Glu10HN	S
Gln9HB-Glu10HN	S
Glu10HA-Ile11HN	M
Glu10HB1-Ile11HA	vW
Glu10HG1-Ile11HG2	M
Glu10HG1-Ile11HD	W
Glu10HN-Ile11HD	S
Ile11HA-Ala12HN	M
Ile11HB-Ala12HN	M
Ile11HG1-Ala12HN	vW
Ile11HG2-Ala12HN	S
Ile11HN-Ala12HB	M
Ala12HA-Ala13HN	M
Ala12HN-Ala13HB	M
Ala13HA-Ile14HN	M
Ala13HB-Ile14HN	S
Ala13HN-Ile14HA	vW
Ala13HN-Ile14HB	W
Ala13HN-Ile14HD	M
Ile14HA-Lys15HN	M
Ile14HG1-Lys15HA	vW
Ile14HD-Lys15HE	M
Lys15HA-Trp16HN	M
Lys15HB1-Trp16HN	M
Lys15HN-Trp16HA	vW
Lys15HN-Trp16HB2	vW
Trp16HA-Glu17HN	W
Trp16HB1-Glu17HN	M
Trp16HB2-Glu17HN	M
Trp16HD1-Glu17HA	W
Trp16HD1-Glu17HN	vW
Trp16HE3-Glu17HA	S
Trp16HE3-Glu17HB1	W
Trp16HE3-Glu17HG1	vW
Trp16HE3-Glu17HN	W
Trp16HZ3-Glu17HB1	vW
Trp16HN-Glu17HB1	vW
Glu17HA-Ile18HD	vW
Glu17HA-Ile18HN	S
Glu17HG1-Ile18HD	W
Glu17HN-Ile18HD	M
Ile18HA-Ala19HN	W
Ile18HB-Ala19HN	M
Ile18HG2-Ala19HA	M
Ile18HG2-Ala19HN	M
Ile18HD-Ala19HN	M
Ile18HN-Ala19HB	M
Ala19HA-Ala20HN	S
Ala19HB-Ala20HN	S
Ala19HN-Ala20HB	W
Ala20HA-Ile21HG2	W
Ala20HA-Ile21HN	M
Ala20HB-Ile21HA	vW
Ala20HB-Ile21HN	S
Ala20HN-Ile21HG2	W
Ala20HN-Ile21HD	vW
Ile21HA-Lys22HN	S
Lys22HA-Gln23HN	S
Lys22HA-Gln23HN22	vW
Lys22HB1-Gln23HN	M
Lys22HB2-Gln23HN	M
Gln23HA-Gly24HN	S
Gly24HA1-Tyr25HD	vW
Gly24HA1-Tyr25HN	S
Gly24HA2-Tyr25HD	vW
Tyr25HA-Gly26HN	M
Tyr25HB1-	vW

Gly26HN	
Tyr25HB2-Gly26HN	vW

Tyr25HD-Gly26HN	vW
Gly26HN-NH_2HN1	vW

HN(i)-HN(i+1)	Intensity
Cp2HN-Glu3HN	M
Glu3HN-Ile4HN	S
Ala5HN-Ala6HN	vS
Lys8HN-Gln9HN	S
Gln9HN-Glu10HN	M
Glu10HN-Ile11HN	S
Ile11HN-Ala12HN	S
Ala12HN-Ala13HN	S
Ala13HN-Ile14HN	S
Lys15HN-Trp16HN	M
Trp16HN-Glu17HN	S
Glu17HN-Ile18HN	S
Ile18HN-Ala19HN	M
Ala19HN-Ala20HN	M/S
Ala20HN-Ile21HN	M/S
Ile21HN-Lys22HN	M
Lys22HN-Gln23HN	M
Tyr25HN-Gly26HN	M

H(i)-H(i+2)	Intensity
Cp2HA-Ile4HN	M
Cp2HB-Ile4HN	M
Ile4HA-Ala6HN	vW
Ile4HN-Ala6HN	M
Ala6HN-Lys8HN	W
Ile7HD-Gln9HN	M
Lys8HA-Glu10HN	M
Glu10HG2-Ala12HN	vW
Ile11HA-Ala13HB	vW
Ile11HA-Ala13HN	vW
Ile11HN-Ala13HN	W

Ala12HB-Ile14HN	W
Ala12HN-Ile14HN	W
Ile14HA-Trp16HN	W
Lys15HA-Glu17HN	M
Trp16HN-Ile18HG2	M
Glu17HN-Ala19HB	vW
Glu17HN-Ala19HN	vW
Ile18HA-Ala20HN	vW
Ala19HB-Ile21HN	W
Ala19HN-Ile21HN	vW
Ala20HB-Lys22HE	vW
Ala20HN-Lys22HN	vW
Ile21HA-Gln23HN	M
Gln23HB-Tyr25HD	vW
Gln23HB-Tyr25HE	vW

H(i)-H(i+3)	Intensity
Cp2HB-Ala5HB	vW
Cp2HB-Ala5HN	S
Cp2HN-Ala5HB	M
Glu3HB2-Ala6HN	vW
Glu3HG-Ala6HB	M
Glu3HG-Ala6HN	vW
Ile4HA-Ile7HG1	M
Ala6HA-Gln9HB	M
Ala6HN-Gln9HN	vW
Ile7HA-Glu10HB1	S
Ile7HA-Glu10HG1	vW
Gln9HA-Ala12HB	S
Gln9HA-Ala12HN	S
Gln9HN-Ala12HB	M

Gln9HN'1-Ala12HB	vW
Glu10HA-Ala13HB	W
Glu10HG2-Ala13HB	M
Ile11HA-Ile14HB	M
Ile11HA-Ile14HG2	M
Ile11HA-Ile14HN	M
Ala12HB-Lys15HA	vW
Ala13HA-Trp16HB1	vW
Ala13HA-Trp16HB2	vW
Ala13HA-Trp16HD1	S
Ala13HA-Trp16HE3	W
Ala13HA-Trp16HN	M
Ala13HB-Trp16HB1	vW
Ala13HB-Trp16HB2	vW
Ala13HB-Trp16HD1	W
Ala13HB-Trp16HE3	vW
Ala13HB-Trp16HH2	vW
Ala13HB-Trp16HZ3	vW
Ala13HB-Trp16HN	W
Ala13HN-Trp16HN	vW
Ile14HA-Glu17HG1	vW
Lys15HA-Ile18HD	M
Trp16HA-Ala19HN	W
Trp16HB1-Ala19HB	vW
Trp16HB2-Ala19HB	vW
Trp16HD1-Ala19HB	W
Trp16HE3-Ala19HB	M
Trp16HH2-Ala19HB	vW
Trp16HZ3-Ala19HA	W

Trp16HN-Ala19HB	W
Trp16HZ3-Ala19HB	vW
Trp16HN-Ala19HN	vW
Glu17HN-Ala20HB	vW
Ile18HA-Ile21HN	M
Ala20HN-Gln23HA	vW
Lys22HA-Tyr25HD	vW
Lys22HA-Tyr25HE	vW
Gly24HA2-NH_2HN1	vW

H(i)-H(i+4)	**Intensity**
Ala5HA-Gln9HN	M
Ile7HN-Ile11HA	vW
Glu10HA-Ile14HN	W
Ala12HA-Trp16HN	M
Ala12HB-Trp16HD1	W
Ala12HB-Trp16HH2	vW
Ala12HB-Trp16HZ3	vW
Ala12HB-Trp16HN	W
Lys15HA-Ala19HN	vW
Trp16HA-Ala20HN	vW
Trp16HD1-Ala20HB	vW
Trp16HH2-Ala20HB	vW
Trp16HZ2-Ala20HB	vW
Trp16HZ3-Ala20HB	vW
Ile18HA-Lys22HN	vW
Ile21HG2-Tyr25HD	M
Ile21HG2-Tyr25HE	M

H(i)-H(i+5)	**Intensity**
Ala20HB-Tyr25HD	vW
Ala20HB-Tyr25HE	vW

Table S3. NMR assignments for peptide **3**.

Residue	Proton	Chemical shift [ppm]
Ac1	HA	2.02
Gly2	HN	8.41
	HA	3.86(2) 4.00(1)
Glu3	HN	8.65
	HA	4.17
	HB	2.39
	HG	1.98(2) 2.05(1)
Ile4	HN	8.16
	HA	3.69
	HB	1.95
	CH2	1.24(2) 1.51(1)
	HG	0.80
	HD	0.74
Ala5	HN	7.62
	HA	3.96
	HB	1.37
Ala6	HN	7.67
	HA	4.12
	HB	1.44
Ile7	HN	8.02
	HA	3.66
	HB	1.98
	CH2	0.95
	HG	0.81
	HD	0.78
Lys8	HN	8.46
	HA	3.76
	HB	1.68(2), 1.84(1)
	HG	1.31
	HD	1.61
	HE	2.85
	NH3Z	7.52
Gln9	HN	7.89
	HA	4.09
	HB	2.16
	HG	2.37(2), 2.47(1)
	HN'	6.76(1), 7.33(2)
Glu10	HN	8.05
	HA	4.14
	HB	2.38(2), 2.60(1)
	HG	1.97(2), 2.38(1)
Ile11	HN	8.49
	HA	3.51
	HB	1.89
	CH2	0.87
	HG	0.79
	HD	0.74
Ala12	HN	7.79
	HA	3.95
	HB	1.43
Ala13	HN	7.67
	HA	4.18
	HB	1.50
Ile14	HN	8.18
	HA	3.67
	HB	1.96
	CH2	0.90
	HG	0.82
	HD	0.78
Lys15	HN	8.54
	HA	3.76
	HB	1.66(2), 1.85(1)
	HG	1.29
	HD	1.55
	HE	2.81
	NH3Z	7.49
Trp16	HN	7.94
	HA	4.35
	HB	3.34(2), 3.48(1)
	HD1	7.21
	HE	7.54
	HZ1	7.05
	HZ2	7.42
	HH	7.15
	HN'	10.04
Glu17	HN	8.17
	HA	3.95
	HB	2.37(2), 2.63(1)
	HG	2.04(2), 2.38(1)
Ile18	HN	8.54
	HA	3.50
	HB	1.77
	CH2	0.83
	HG	0.76
	HD	0.64
Ala19	HN	7.64
	HA	3.92
	HB	1.35
Ala20	HN	7.45
	HA	3.97
	HB	1.19
Ile21	HN	7.64
	HA	3.64
	HB	1.79
	CH2	0.82
	HG	0.75
	HD	0.64
Lys22	HN	8.01
	HA	3.85
	HB	1.65(2), 1.73(1)
	HG	1.28(2), 1.42(1)
	HD	1.47(2), 1.55(1)
	HE	2.83
	NH3Z	7.50
Cp23	HN	7.31
	HA	2.54
	HB	4.13
	HG,D,E	1.64(3), 1.70(2), 1.95(1)
Gly24	HN	7.98
	HA	3.74(2), 3.85(1)
Tyr25	HN	8.10
	HA	4.51
	HB	2.87(2), 3.09(1)
	HD	7.04
	HE	6.69
Gly26	HN	8.25
	HA	3.73(2), 3.85(1)
NH2	HN1	7.24
	HN2	7.09

H(i)-H(i+1)	**Intensity**
Ac1HA-Gly2HN	S
Gly2HA1-Glu3HN	S
Gly2HA2-Glu3HN	S
Glu3HN-Ile4HG	W
Glu3HA-Ile4HN	S
Glu3HN-Ile4HD	W
Ile4HA-Ala5HN	M
Ile4HB-Ala5HN	S
Ile4HG-Ala5HN	M
Ile4HN-Ala5HB	M
Ala5HA-Ala6HN	S
Ala5HB-Ala6HA	W
Ala5HB-Ala6HN	S
Ala5HN-Ala6HA	W
Ala6HA-Ile7HN	M
Ala6HB-Ile7HN	S
Ile7HA-Lys8HN	M
Ile7HB-Lys8HN	S
Ile7CH2-Lys8HB1	M
Ile7HD-Lys8HE	M
Lys8HA-Gln9HN	M
Lys8HB-Gln9HN	W
Lys8HB1-Gln9HN	S
Lys8HN-Gln9HB	W
Gln9HA-Glu10HN	S
Gln9HB-Glu10HN	S
Glu10HA-Ile11HN	M
Glu10HB1-Ile11HN	W
Glu10HB2G1-Ile11HN	M/S
Glu10HG2-Ile11HA	S
Glu10HG2-Ile11HN	M
Glu10HN-Ile11HA	W
Ile11HB-Ala12HN	S
Ile11HN-Ala12HB	M
Ile11HA-Ala12HN	M
Ala12HA-Ala13HN	S
Ala12HN-Ala13HB	M
Ala12HN-Ala13HA	W
Ala13HA-Ile14HN	S/M
Ala13HB-Ile14HN	S
Ala13HN-Ile14HB	M
Ile14CH2-Lys15HB1	S
Ile14HA-Lys15HN	M
Ile14HB-Lys15HN	S
Ile14HN-Lys15HB1	S
Ile14HD-Lys15HA	M
Ile14HD-Lys15HE	M
Lys15HN-Trp16HB2	W
Lys15HB1-Trp16HN	S
Lys15HN-Trp16HA	W
Trp16HA-Glu17HN	M
Trp16HE3-Glu17HB1	W
Trp16HB1-Glu17HN	S
Trp16HB2-Glu17HN	M/S
Trp16HE3-Glu17HN	W
Trp16HE3-Glu17HB2G1	M
Trp16HD1-Glu17HA	W/M
Trp16HE3-Glu17HA	S
Trp16HN-Glu17HA	M
Trp16HZ3-Glu17HA	W
Glu17HA-Ile18HN	S
Glu17HB2G1-Ile18HA	W
Glu17HB2G1-Ile18HN	M/S
Glu17HA-Ile18HG	M
Glu17HB1-Ile18HG	M
Glu17HG2-Ile18HN	W/M
Ile18HN-Ala19HA	S
Ile18HA-Ala19HN	W/M
Ile18HB-Ala19HA	W
Ala19HA-Ala20HN	M
Ala19HB-Ala20HN	S
Ala20HA-Ile21HN	S
Ala20HB-Ile21HN	S
Ala20HN-Ile21HA	W
Ile21HA-Lys22HN	S
Ile21HB-Lys22HN	S
Ile21HN-Lys22HB1	S
Ile21HD-Lys22HA	W
Ile21HD-Lys22HB1	S
Ile21HD-Lys22HE	W
Ile21HD-Lys22HN	M/S
Ile21HN-Lys22HA	W
Lys22HA-Cp23HN	M
Cp23HA-Gly24HN	S
Cp23HB-Gly24HN	W/M
Gly24HA1-Tyr25HN	S
Gly24HA2-Tyr25HD	W
Gly24HA2-Tyr25HE	W
Gly24HA2-Tyr25HN	M
Tyr25HA-Gly26HN	S
Tyr25HB1-Gly26HA1	W
Tyr25HB1-Gly26HN	W
Tyr25HD-Gly26HA1	S
Tyr25HE-Gly26HA1	W
Tyr25HB2-Gly26HA1	W
Tyr25HB2-Gly26HN	W
Gly26HA1-NH2HN1	W

HN(i)-HN(i+1)	Intensity
Gly2HN-Glu3HN	M
Glu3HN-Ile4HN	S
Ile4HN-Ala5HN	S
Ala5HN-Ala6HN	S
Ala6HN-Ile7HN	S
Ile7HN-Lys8HN	S
Lys8HN-Gln9HN	S
Gln9HN-Glu10HN	S
Glu10HN-Ile11HN	S
Ile11HN-Ala12HN	S
Ala13HN-Ile14HN	S
Ile14HN-Lys15HN	S
Lys15HN-Trp16HN	S
Trp16HN-Glu17HN	S
Glu17HN-Ile18HN	S
Ile18HN-Ala19HN	S
Ala20HN-Ile21HN	S
Lys22HN-Cp23HN	S
Cp23HN-Gly24HN	M
Gly24HN-Tyr25HN	M
Tyr25HN-Gly26HN	S

H(i)-H(i+2)	Intensity
Gly2HA2-Ile4HN	W/M
Glu3HA-Ala5HN	W/M
Glu3HN-Ala5HB	W
Glu3HN-Ala5HN	W
Ala5HA-Ile7HN	W/M
Ala5HB-Ile7HN	M
Ala6HB-Lys8HN	M
Ala6HN-Lys8HN	W
Ile7HD-Gln9HN	W
Ile7HA-Gln9HG2	S
Lys8HA-Glu10HN	W/M
Glu10HA-Ala12HN	W/M
Ile11HA-Ala13HN	M
Ile11HN-Ala13HB	W
Ile11HN-Ala13HN	W
Ala12HN-Ile14CH2	W
Ala12HB-Ile14HN	M/S
Ala12HN-Ile14HD	M/S
Ala12HN-Ile14HN	W
Ala13HA-Lys15HN	W
Ala13HB-Lys15HN	W/M
Ile14HA-Trp16HE3	W
Lys15HA-Glu17HN	W/M
Lys15HB1-Glu17HA	M
Trp16HZ2-Ile18HN	W
Trp16HN-Ile18HG	W
Ile18HA-Ala20HN	W
Ile18HB-Ala20HN	W/M
Ala20HN-Lys22HN	W
Ile21HA-Cp23HN	W
Ile21HN-Cp23HN	W
Cp23HA-Tyr25HN	W

H(i)-H(i+3)	Intensity
Gly2HN-Ala5HB	M
Glu3HN-Ala6HB	W
Glu3HB-Ala6HB	M
Glu3HN-Ala6HN	W
Ala5HA-Lys8HN	M/S
Ala5HB-Lys8HN	W/M
Ala6HB-Gln9HB	W/M
Ala6HN-Gln9HN	W
Ile7HA-Glu10HB1	W
Gln9HA-Ala12HN	S
Gln9HN-Ala12HB	M
Gln9HN-Ala12HN	W/M
Glu10HB2G1-Ala13HN	W
Glu10HB2G1-Ala13HB	M
Ile11HN-Ile14HN	W/M
Ala12HB-Lys15HN	W
Ala12HN-Lys15HA	W/M
Ala13HA-Trp16HD1	M
Ala13HA-Trp16HE3	M
Ala13HA-Trp16HN	M
Ala13HB-Trp16HB1	
Ala13HB-Trp16HB2	W
Ala13HB-Trp16HD1	W
Ala13HN-Trp16HN	M
Ala13HA-Trp16HB1	W
Ala13HA-Trp16HB2	W
Ile14HA-Glu17HG2	M
Trp16HA-Ala19HN	M
Trp16HB1-Ala19HB	W
Trp16HB2-Ala19HB	W
Trp16HD1-Ala19HB	W/M
Trp16HE3-Ala19HB	M
Trp16HN-Ala19HB	W
Ile18HA-Ile21HD	S
Ala19HA-Lys22HB2	W
Ala20HA-Cp23HN	M
Ile21HB-Gly24HA2	M/S
Cp23HB-NH2HN1	W/M

H(i)-H(i+4)	Intensity
Ac1HA-Ala5HN	W
Ile4HD-Lys8HA	S
Ile4HA-Lys8HB1	M/W
Ala5HA-Gln9HN	W/M
Ala12HB-Trp16HD1	W
Ala12HB-Trp16HN	W
Lys15HA-Ala19HN	W/M
Trp16HA-Ala20HN	W
Trp16HE3-Ala20HB	M
Glu17HB1-	W

Ile21HD	
Glu17HB2G1-Ile21HD	W/M
Ile18HA-Lys22HN	W
Ile21HD-Tyr25HD	M
Ile21HD-Tyr25HE	M

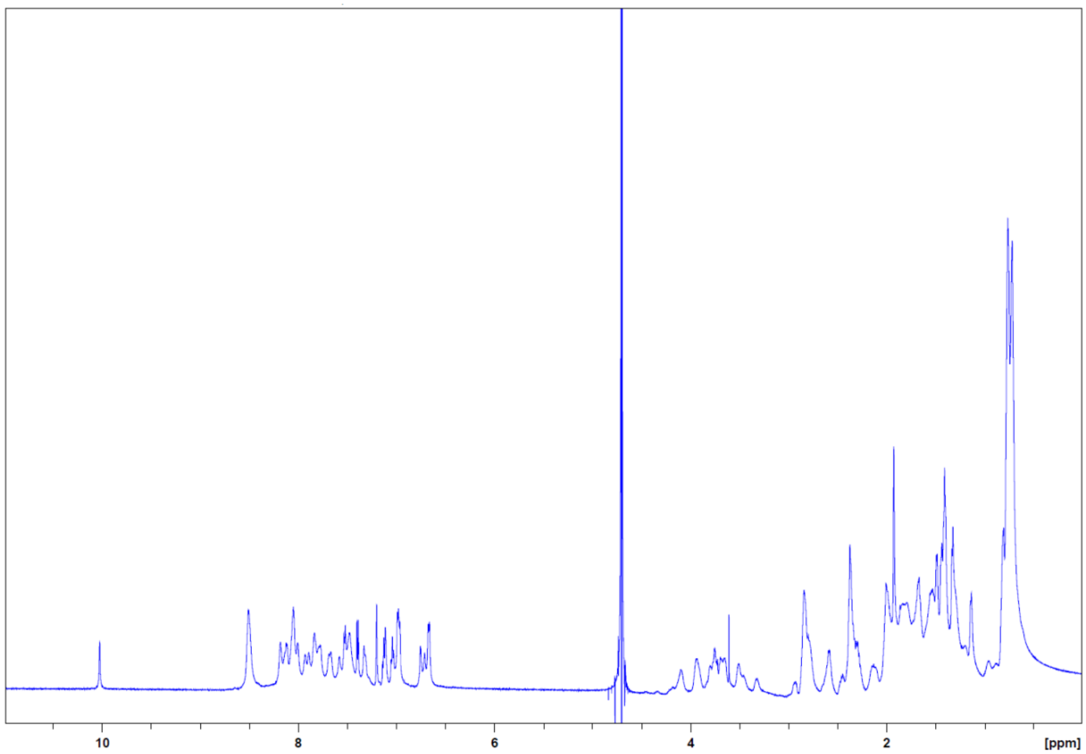


Fig. S4. 1D ^{1}H NMR spectrum recorded for peptide **2** dissolved in D_2O/H_2O (pH=7) at 298 K.

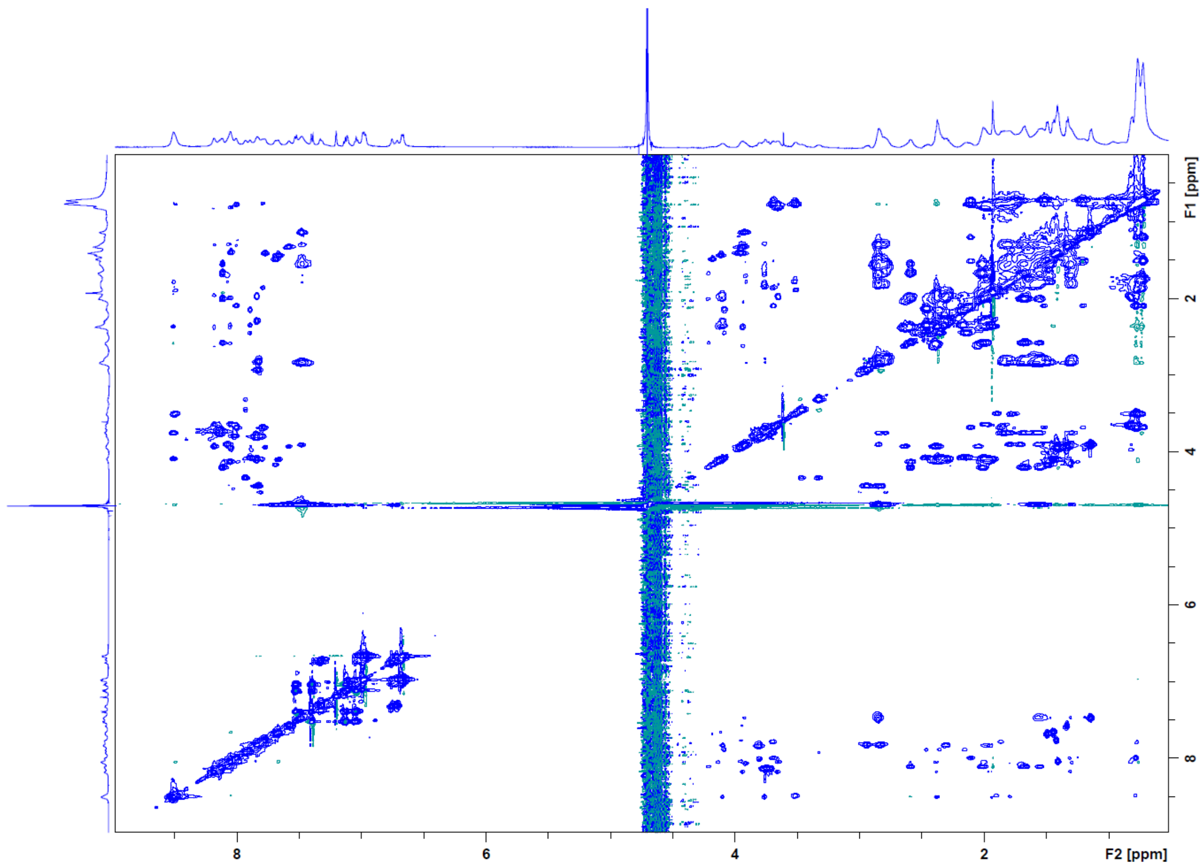


Fig. S5. 2D TOCSY spectrum recorded for peptide **2** dissolved in D_2O/H_2O (pH=7) at 298 K.

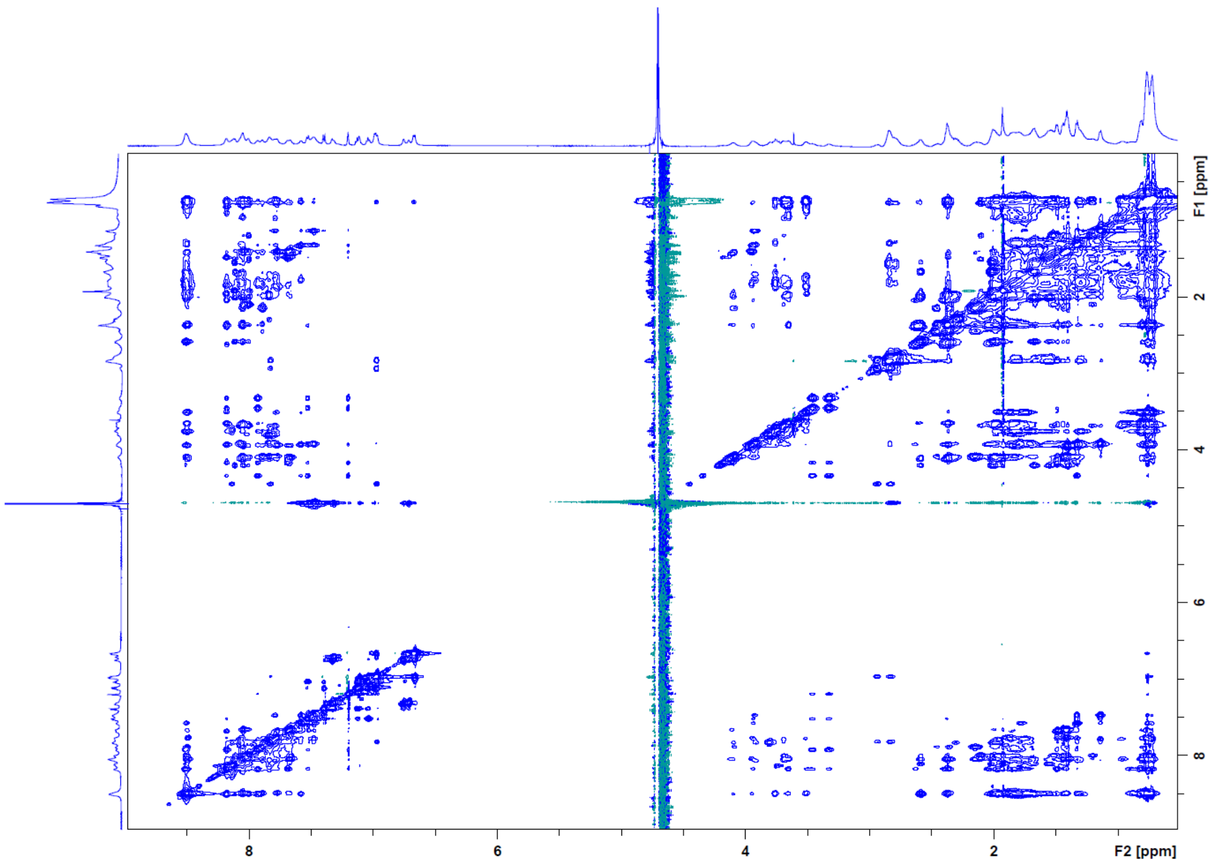


Fig. S6. 2D NOESY spectrum recorded for peptide **2** dissolved in D_2O/H_2O (pH=7) at 298 K.

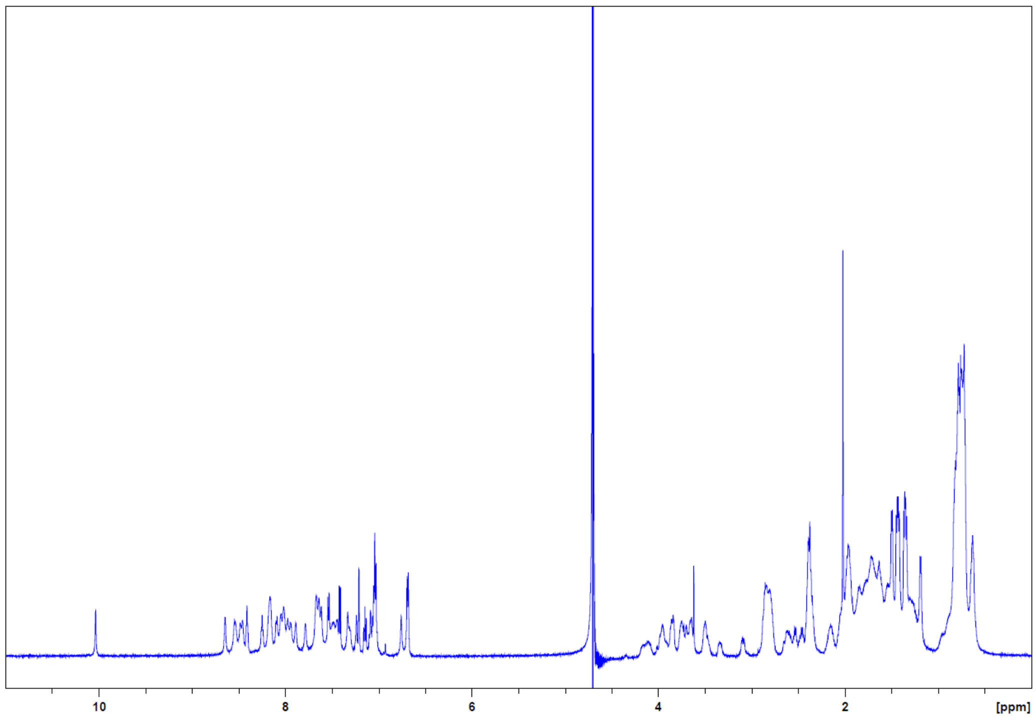


Fig. S7. 1D ^{1}H NMR spectrum recorded for peptide **3** dissolved in D_2O/H_2O (pH=7) at 298 K.

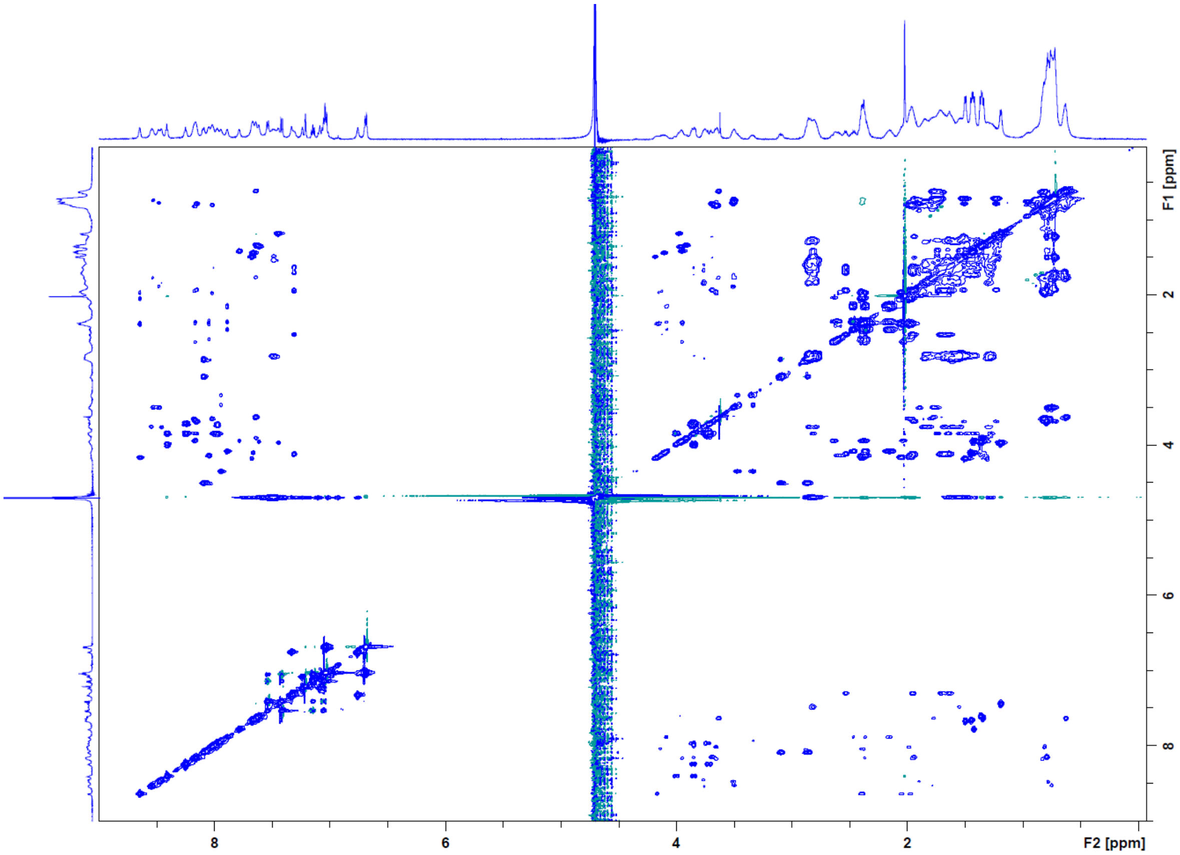


Fig. S8. 2D TOCSY spectrum recorded for peptide **3** dissolved in D_2O/H_2O (pH=7) at 298 K.

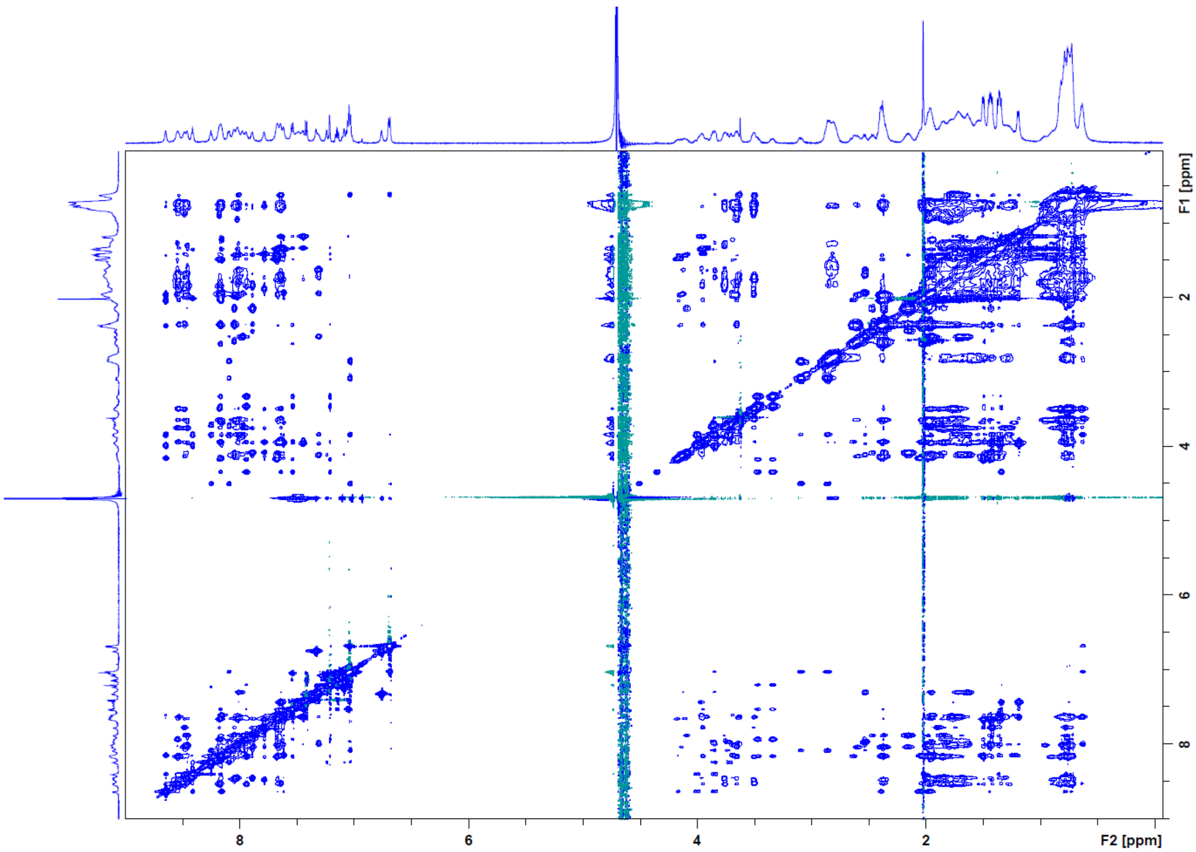


Fig. S9. 2D NOESY spectrum recorded for peptide **3** dissolved in D_2O/H_2O (pH=7) at 298 K.

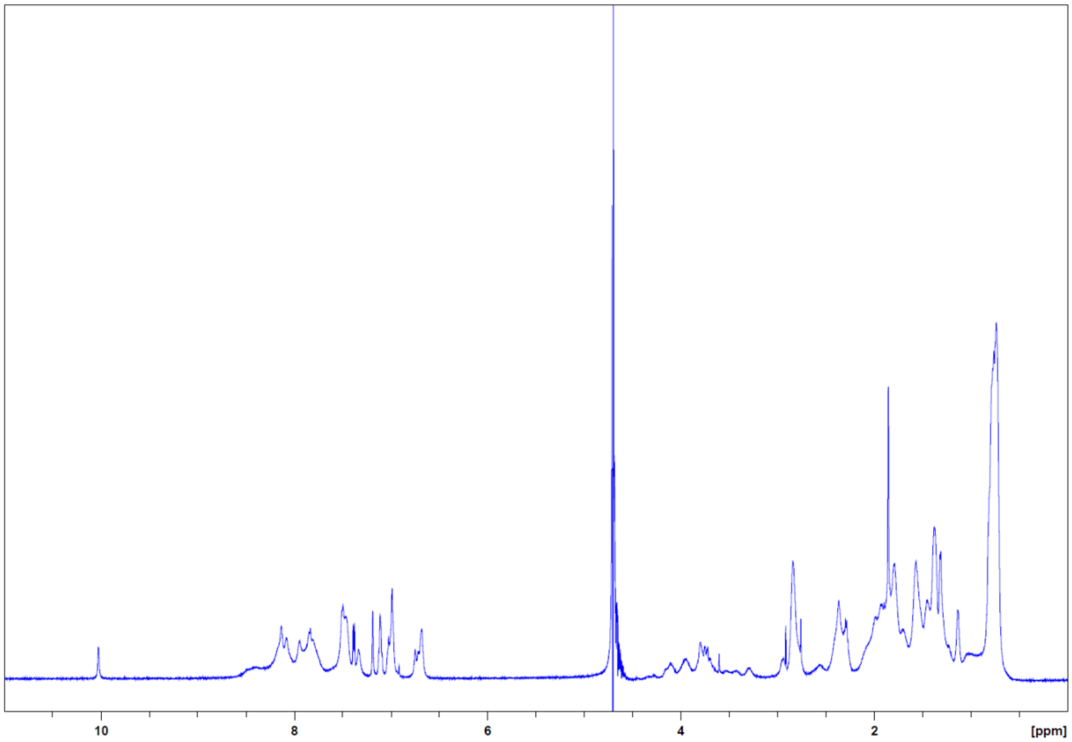


Fig. S10. 1D ^{1}H NMR spectrum recorded for peptide **5** dissolved in D_2O/H_2O (pH=7) at 298 K.

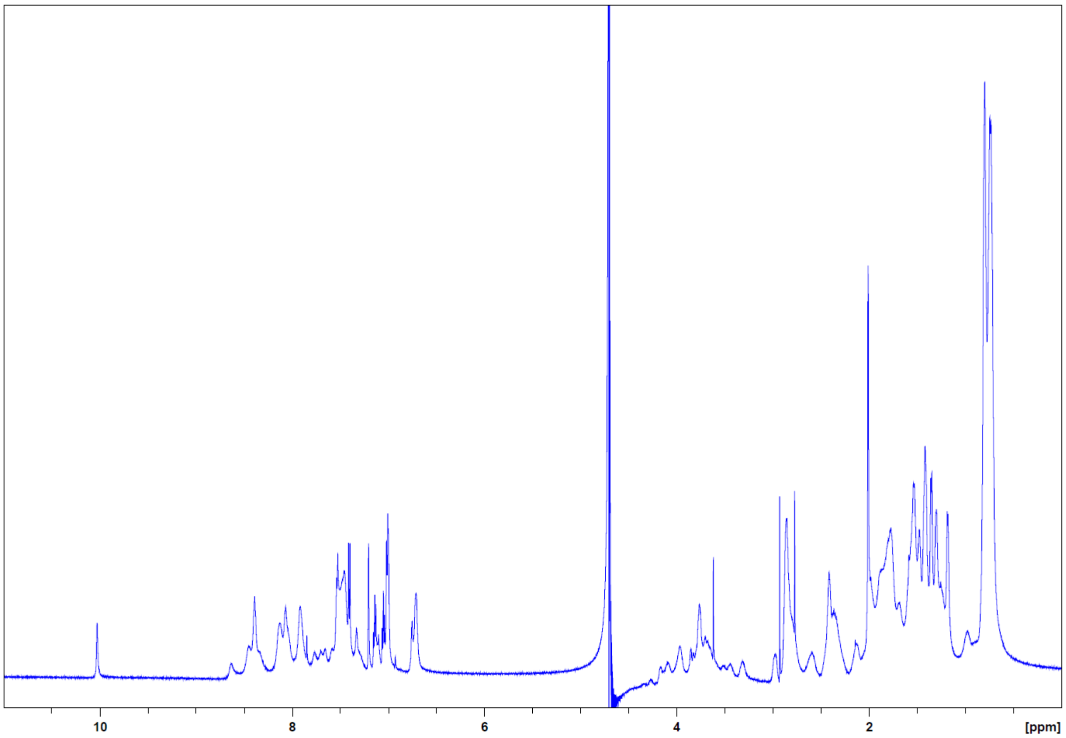
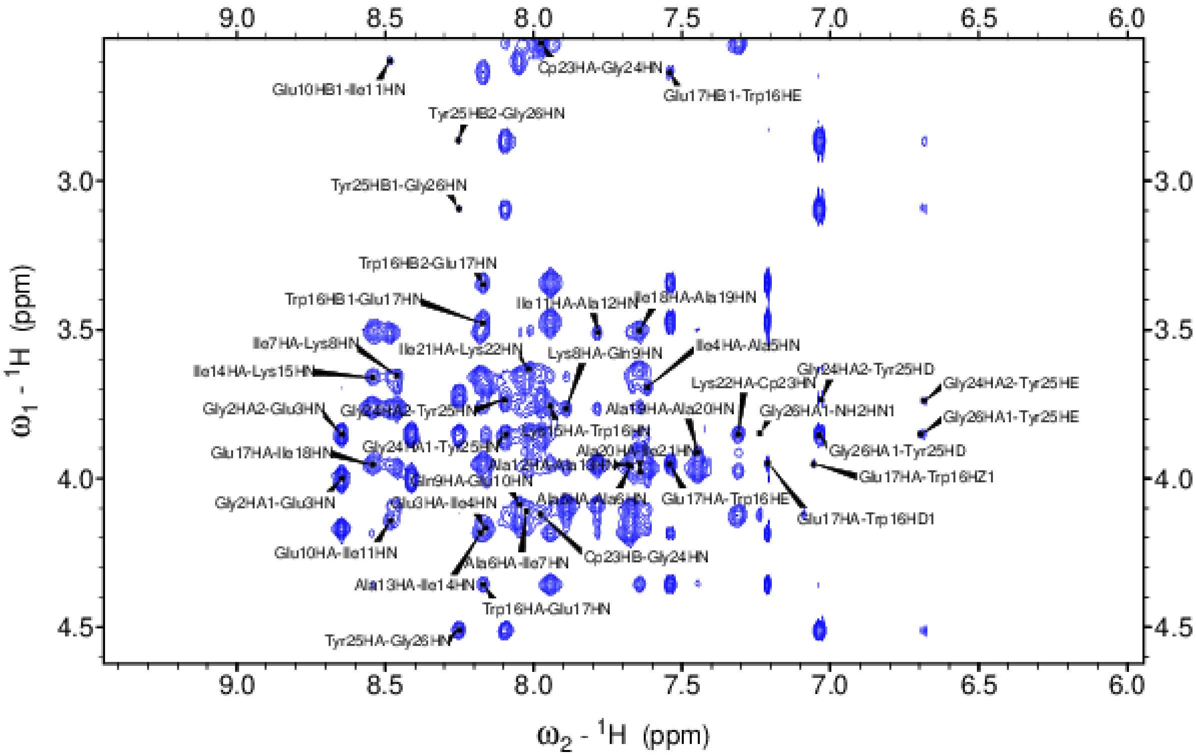


Fig. S11. 1D ^{1}H NMR spectrum recorded for peptide **6** dissolved in D_2O/H_2O (pH=7) at 298 K.

A



B

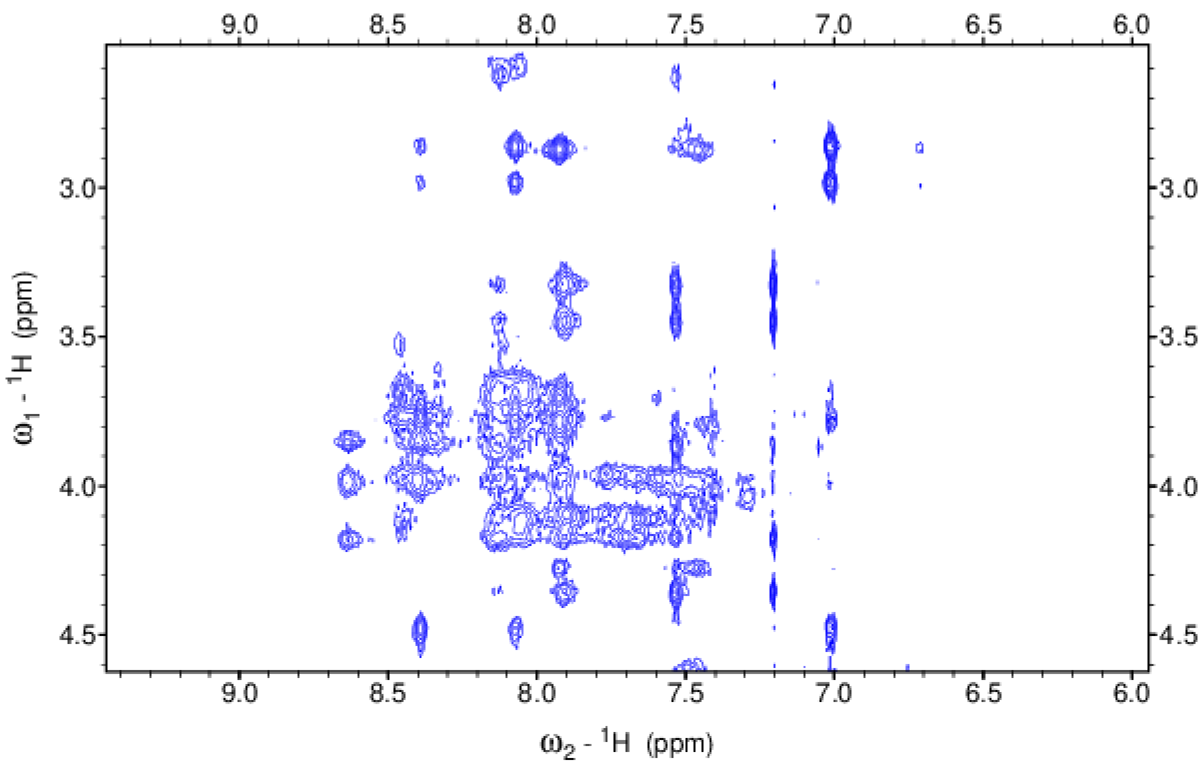


Fig. S12. Selected fragments of 2D NOESY spectra region recorded for peptide **3** (A) and **6** (B) dissolved in D_2O/H_2O (pH=7) at 298 K.

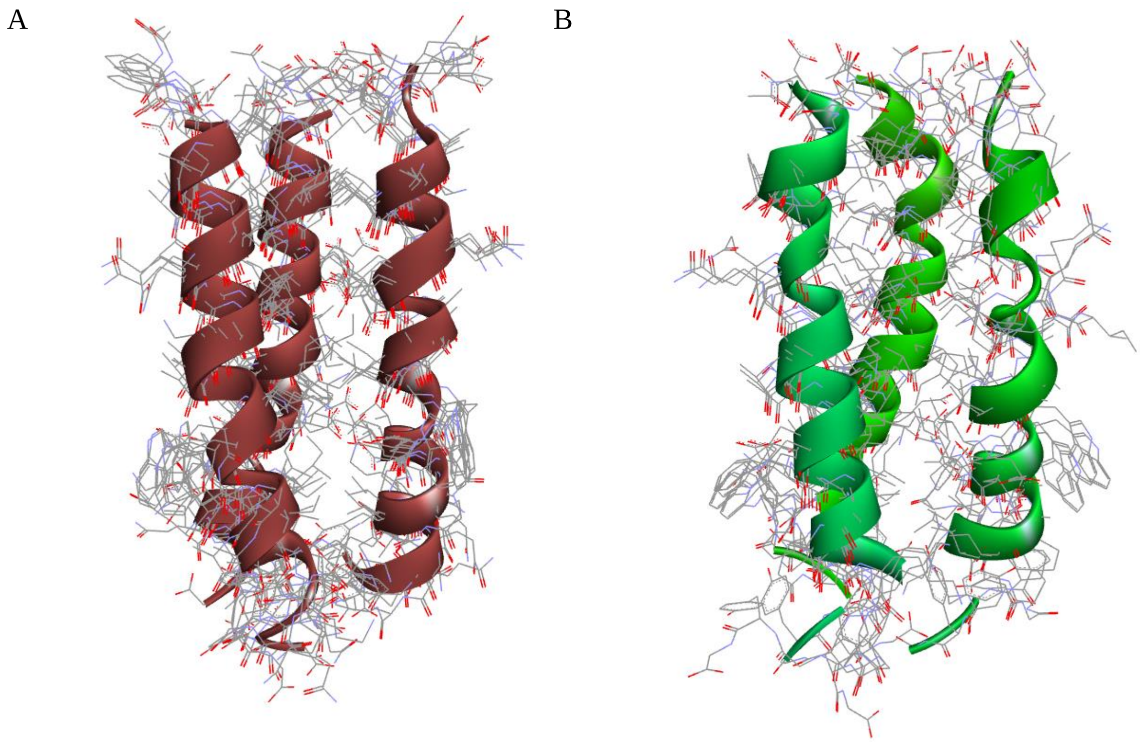


Fig. S13. Superimposition of the five lowest energy structures calculated on the basis of restraints derived from 2D NOESY for peptide **2** (A) and **3** (B). For the clarity, one of them is additionally showed in a solid ribbon representation.

Table S4. Statistic of the calculations for peptides **2** and **3** averaged over 10 lowest energy structures.

Peptide	**2**	**3**
Total number of NOE restraint from NMR	208	201
Applied number of intrahelical NOE restraint	159	166
(i, i+1)	89	102
(i, i+2)	20	22
(i, i+3)	37	29
(i, i+4)	11	13
(i, i+5)	2	0
Applied number of interhelical NOE	8 · 3	10 · 3
Total number of different NOE violations in ensemble	44	56
Average number of NOE violations per structure	7.8	8.3
Average amount of NOE violation per structure [Å]	5.4	5.7
Total number of different VdW violations in ensemble	19	15
Average number of VdW violations per structure	3.5	3.5
Average amount of VdW violation per structure [Å]	0.8	0.8
Average RMSD for backbone heavy atoms [Å]	2.3	3.1
Average RMSD for all heavy atoms [Å]	2.8	3.3