Conformational stabilization of a β-hairpin through a triazole-tryptophan interaction

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Experimental procedure

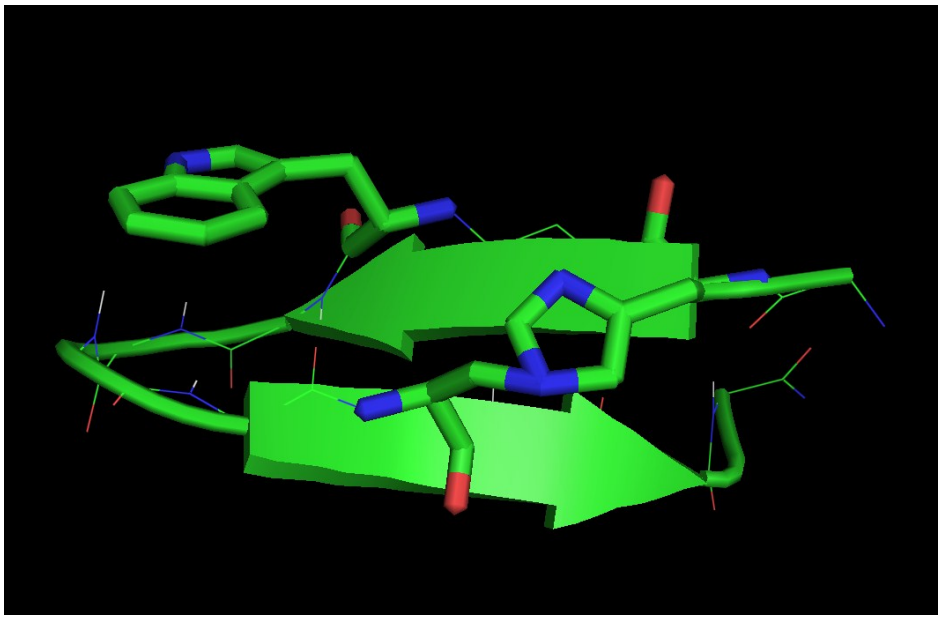
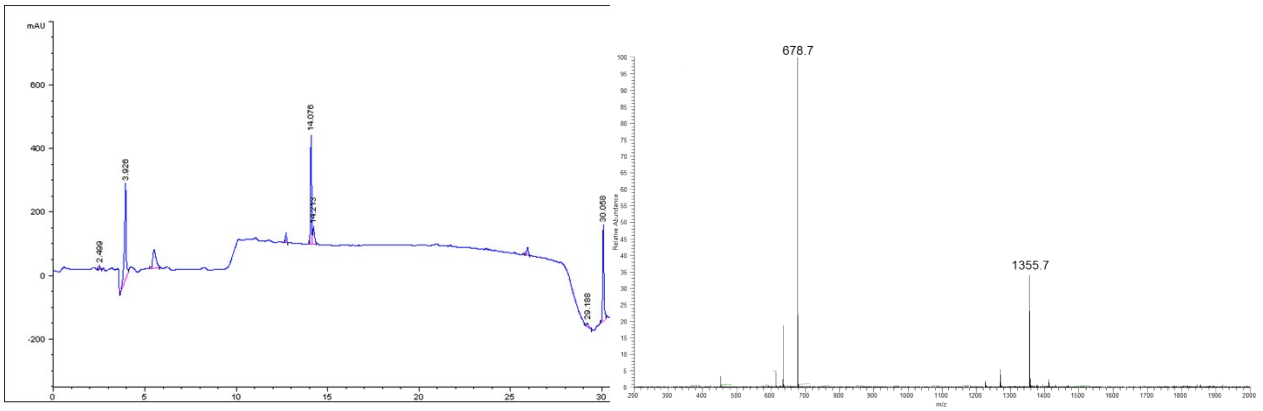
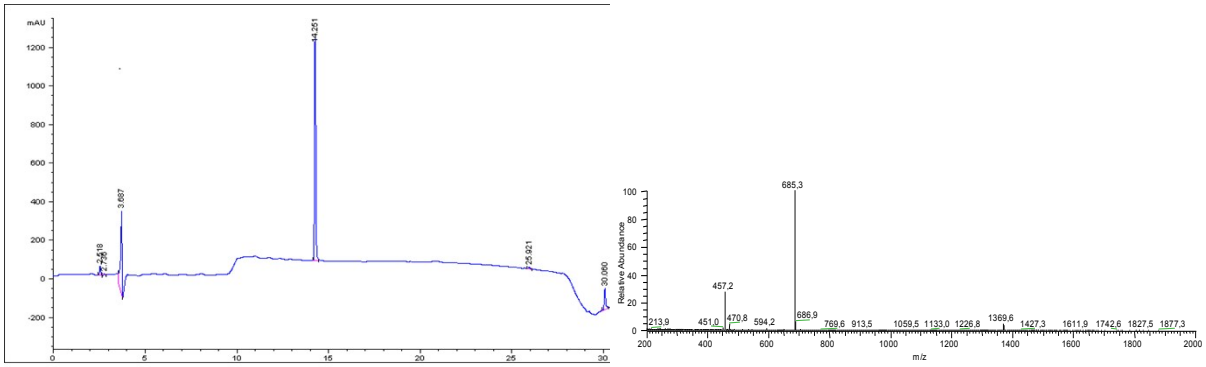


Figure S1: Schematic representation of DNHB peptides. The key elements, Trp and triazole bridge, are reported. The figure was prepared using Pymol software.

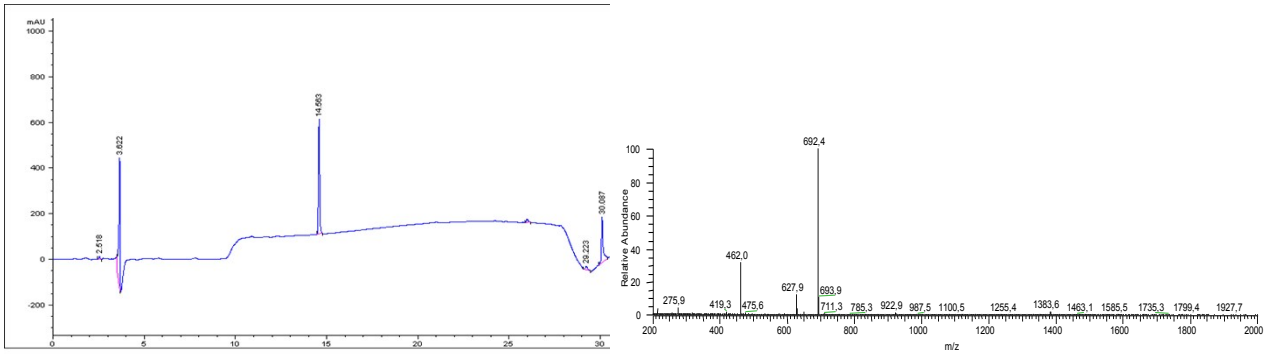
DNHB 1.1 linear



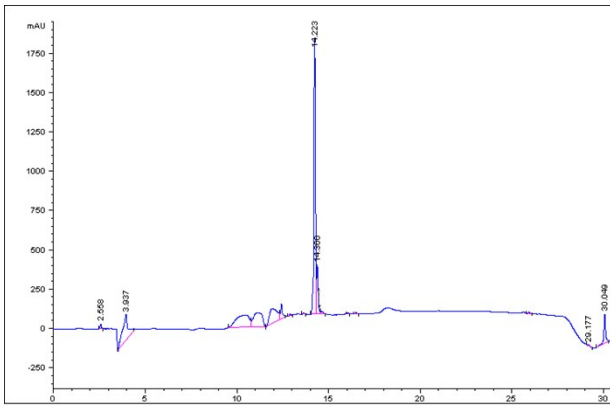
DNHB 1.2 linear

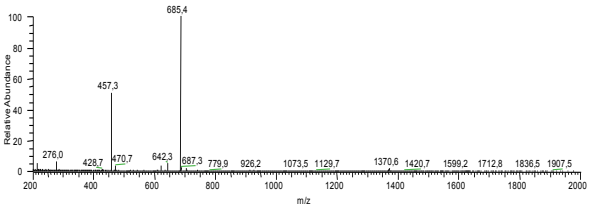


DNHB 1.3 linear



DNHB 2.1 linear





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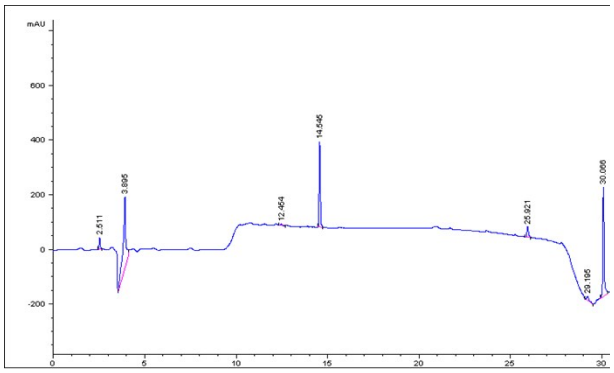

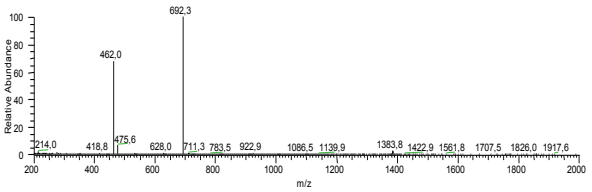

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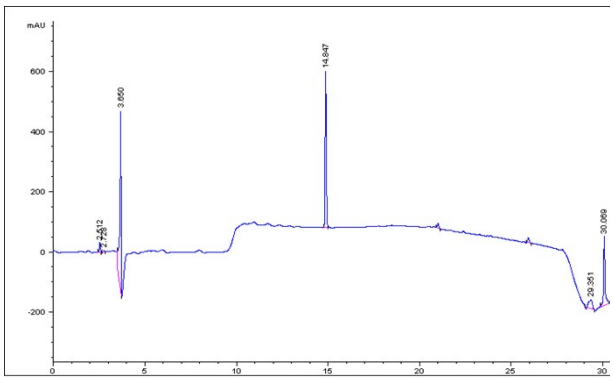
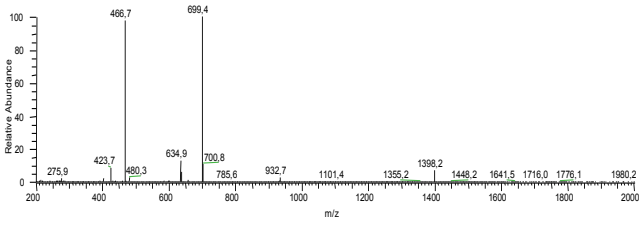
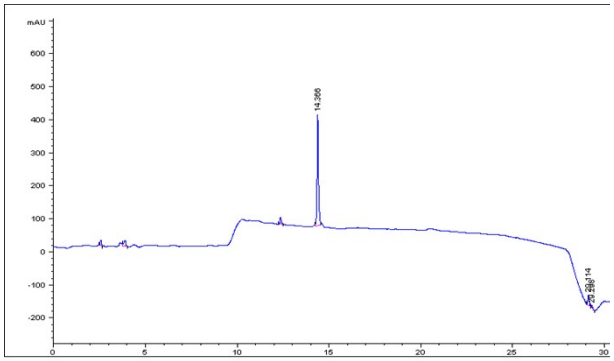
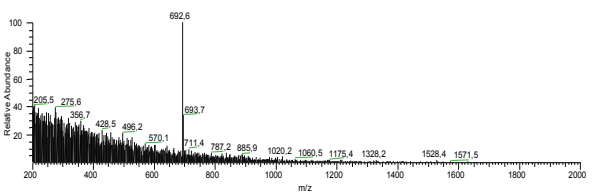




DNHB 3.1 linear





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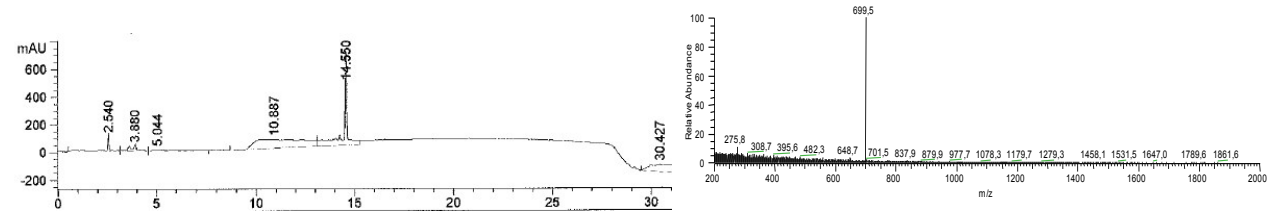
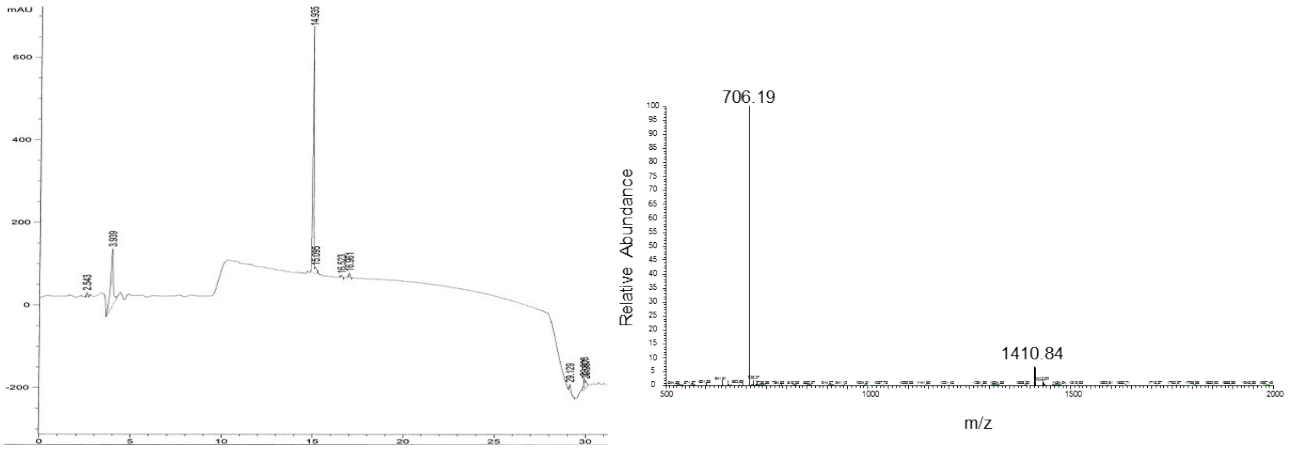
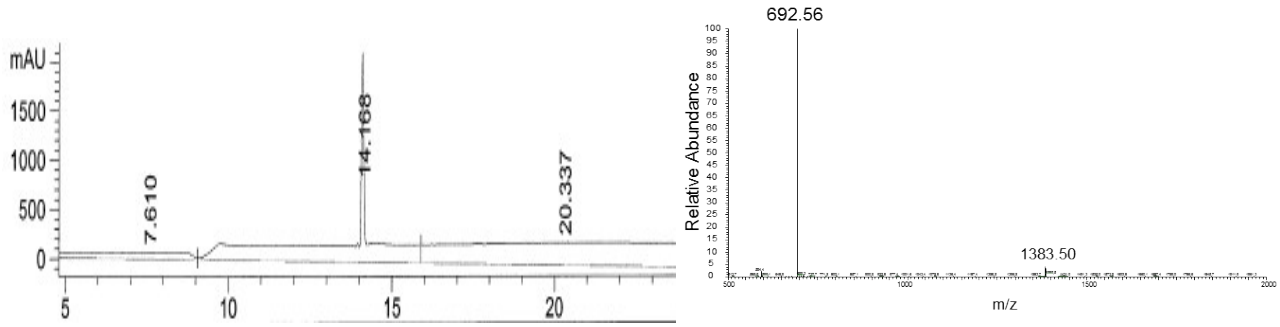


DNHB 3.3 linear



DNHB 2.2W3linear



DNHB 2.2rev linear

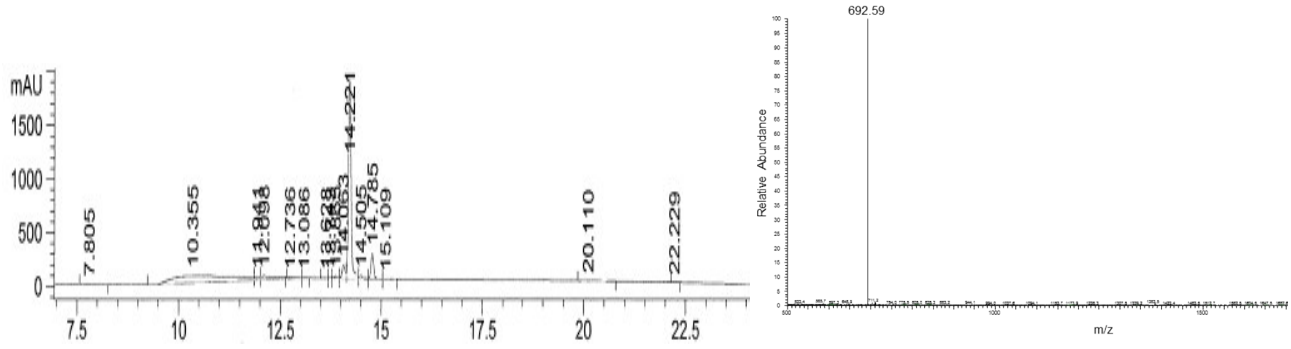
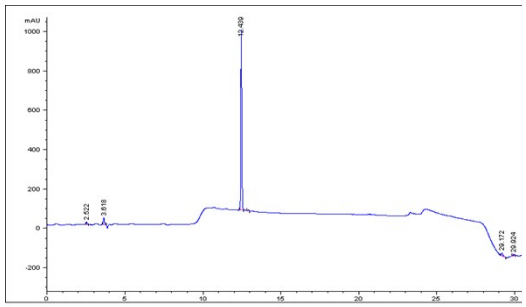
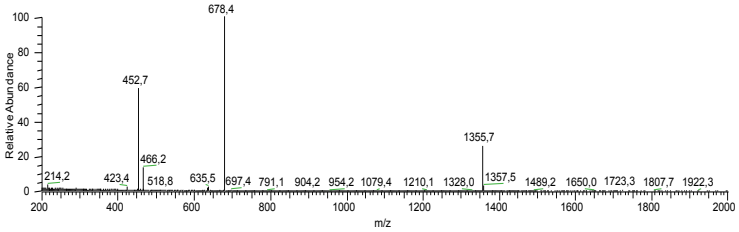


Figure S2: Chromatographic RP-HPLC profile revealing at 210 nm and ESI-MS spectrum of the linear DNHB peptides.

DNHB 1.1





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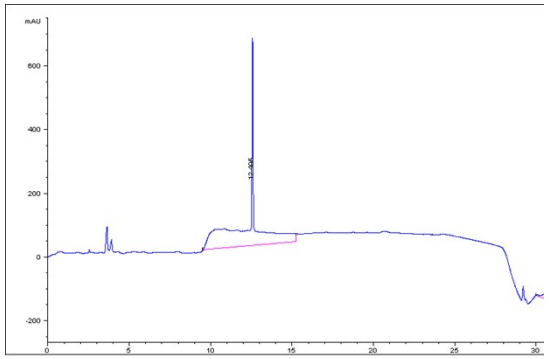
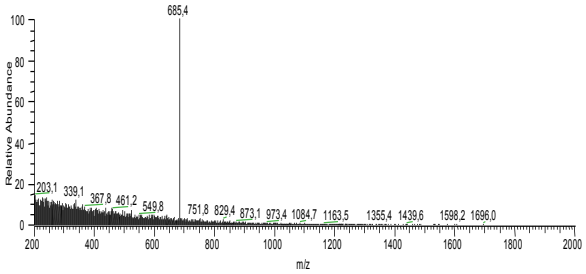
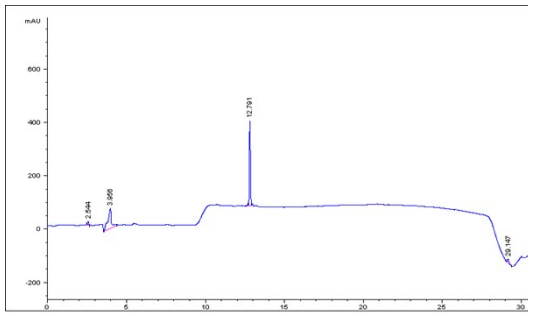
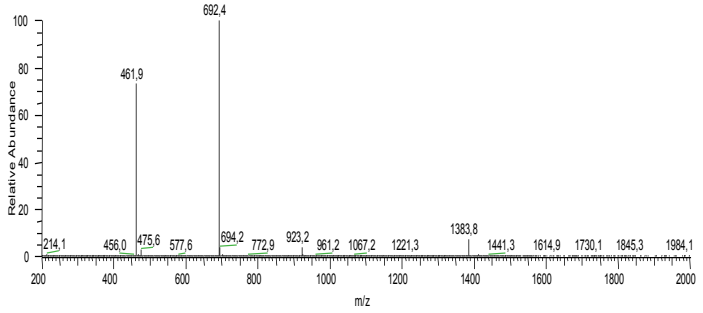


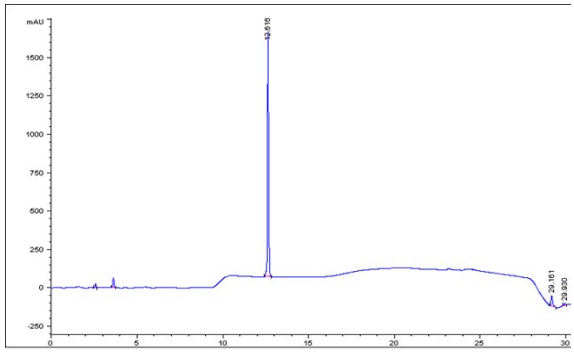


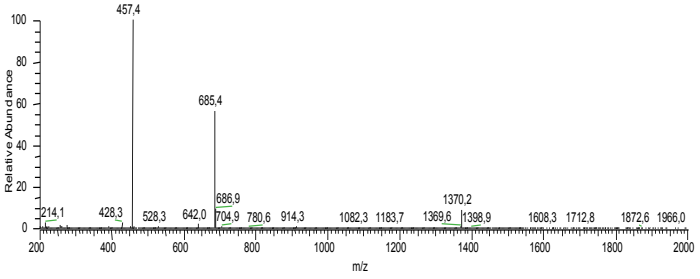
DNHB 1.3





DNHB 2.1





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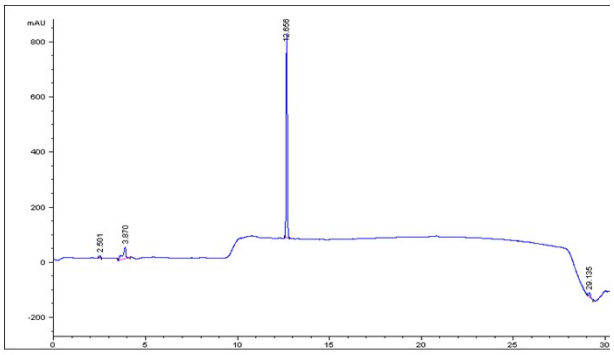

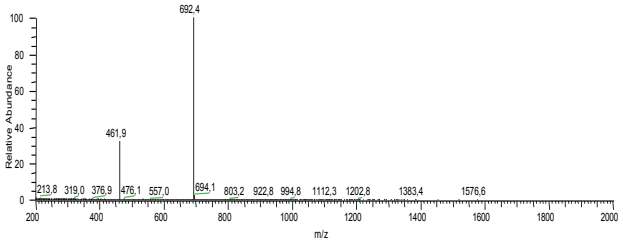

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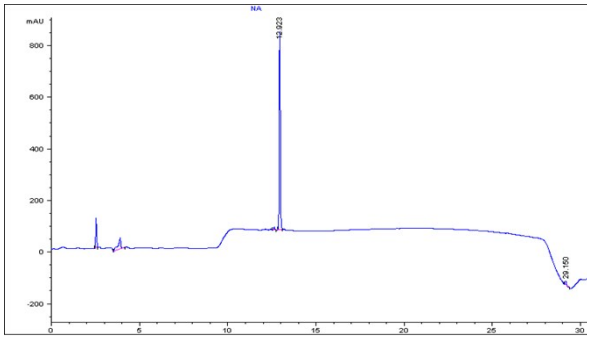
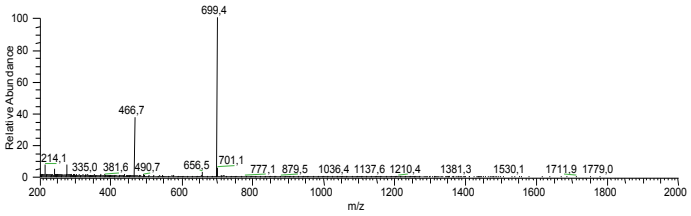
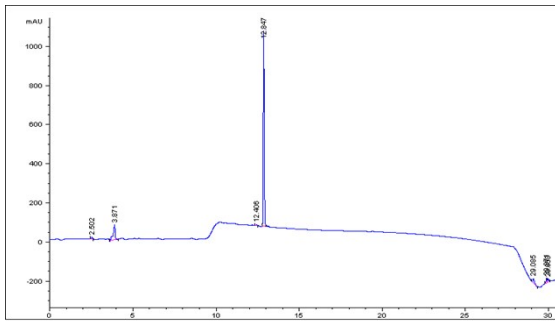
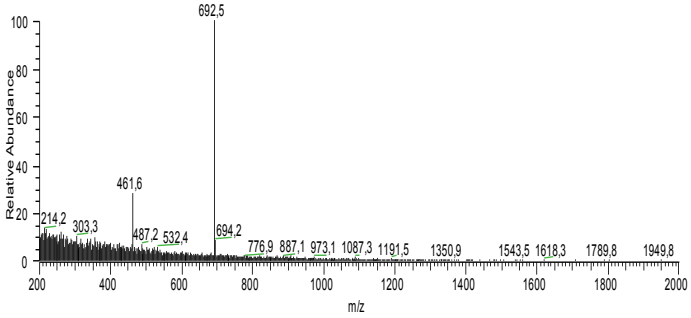




DNHB 3.1





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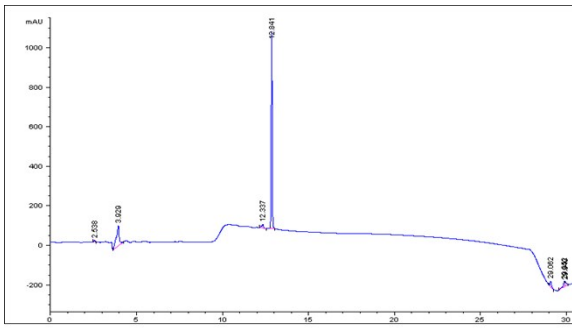
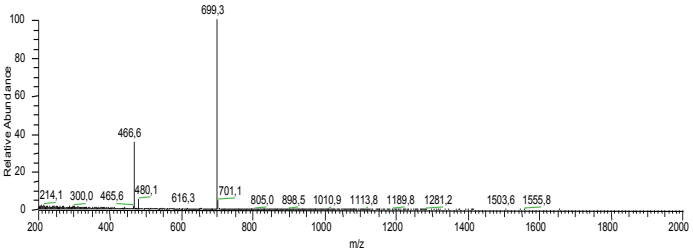
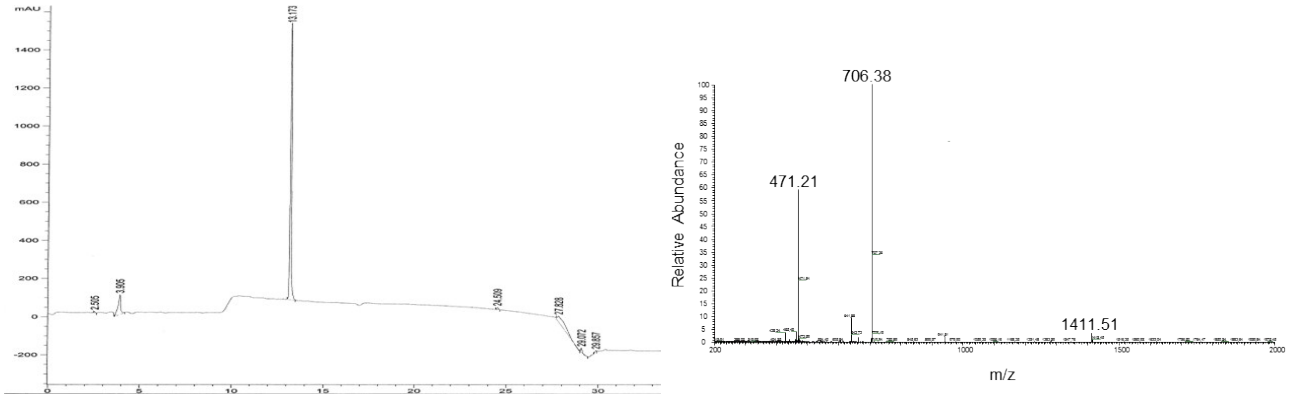
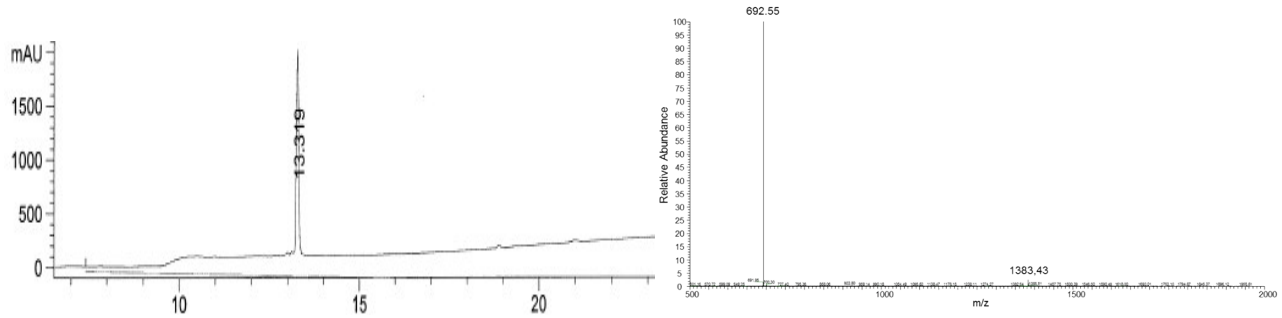




DNHB 3.3



DNHB 2.2W3



DNHB 2.2rev

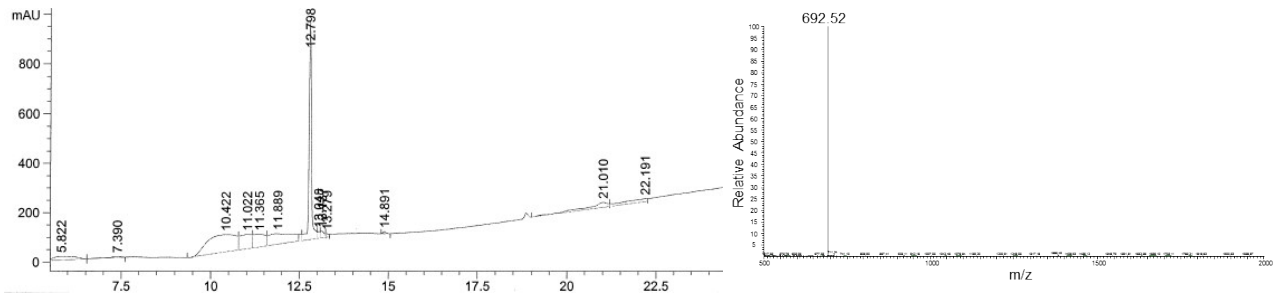


Figure S3: Chromatographic RP-HPLC profile revealing at 210 nm and ESI-MS spectrum of the cyclic DNHB peptides.

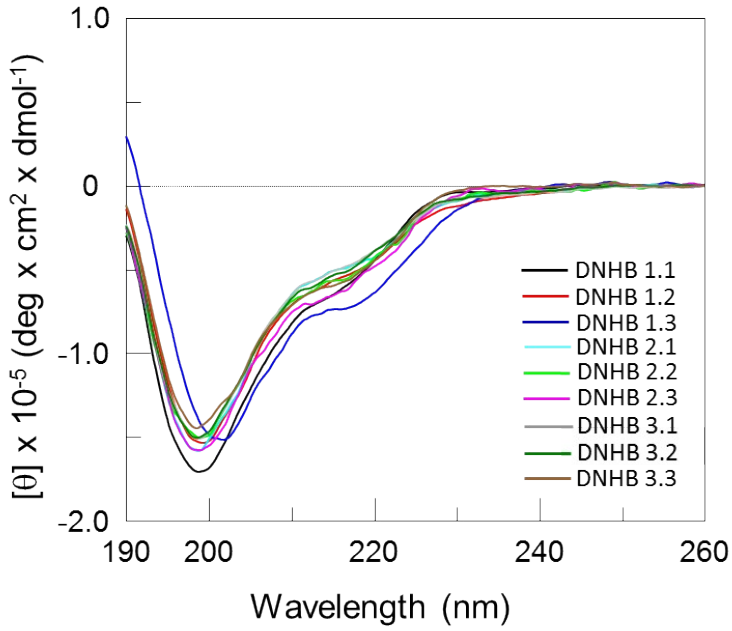


Figure S4: Far-UV circular dichroism spectra of linear DNHB peptides in 10 mM phosphate buffer pH 6.6. Spectra are reported as molar ellipticity ([θ]).

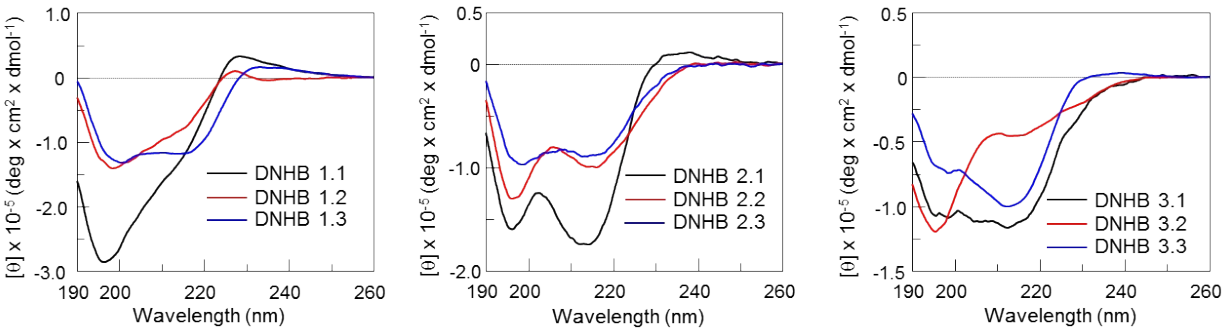


Figure S5: Far-UV circular dichroism spectra of DNHB peptides in 10 mM phosphate buffer pH 6.6. Spectra are reported as molar ellipticity ([θ]).

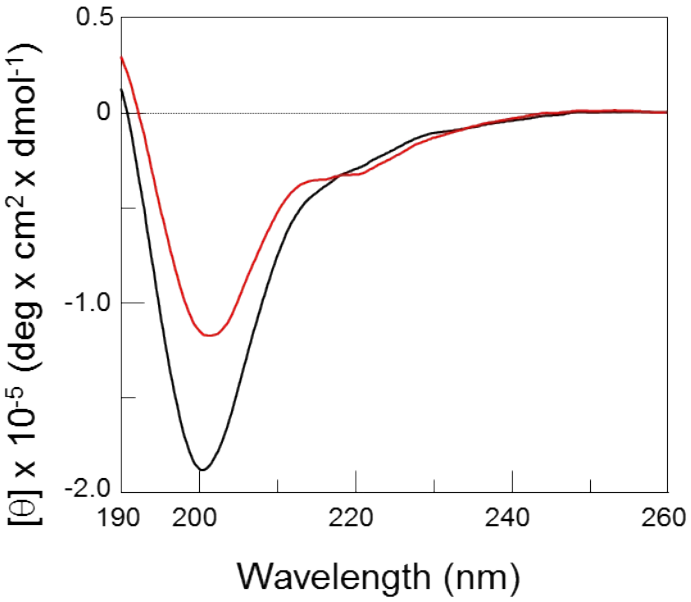


Figure S6: Far-UV circular dichroism spectra of linear (black line) and cyclized (red line) DNHB2.2W3 peptides in 10 mM phosphate buffer pH 6.6. Spectra are reported as molar ellipticity ([θ]).

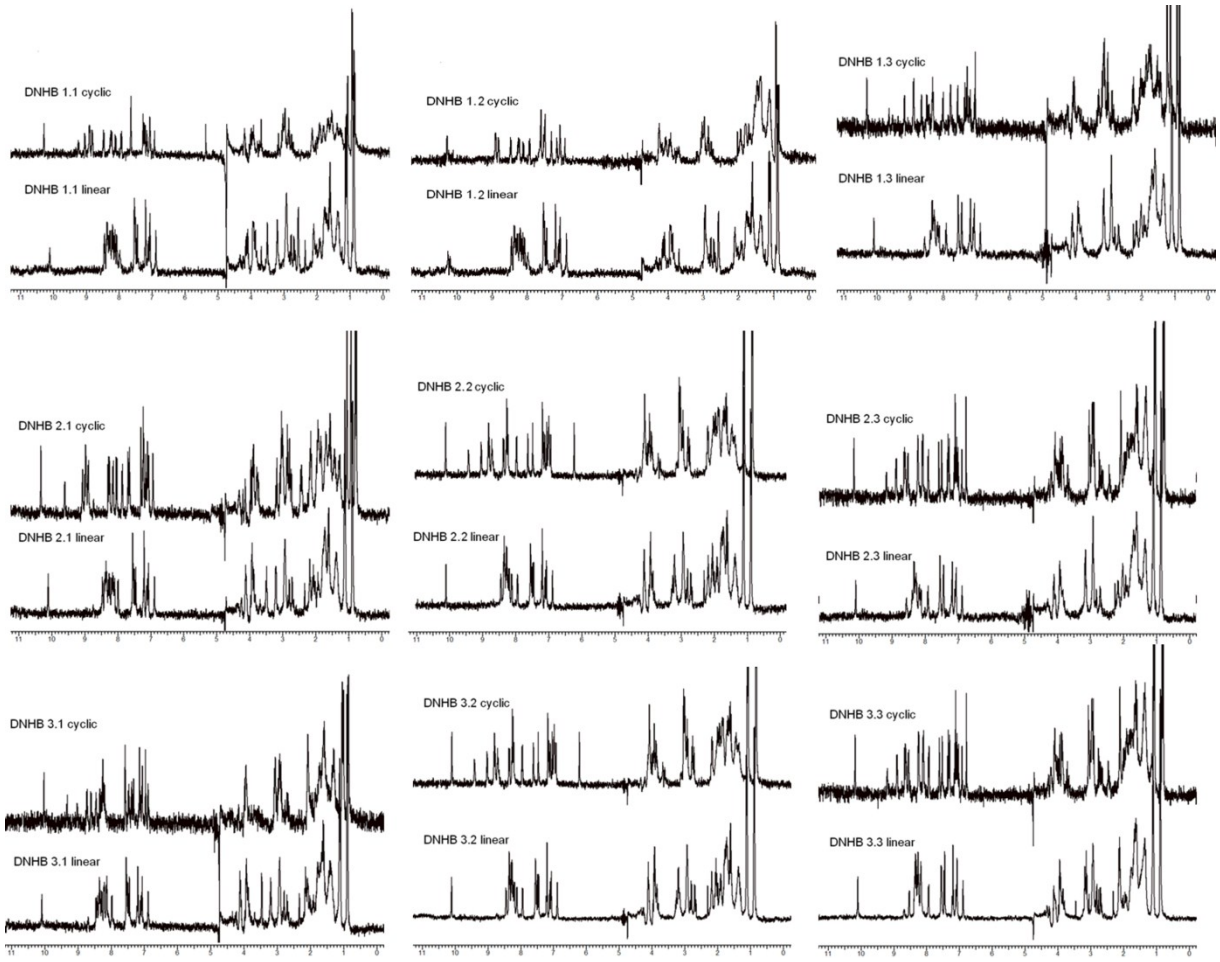


Figure S7 : One-dimensional proton spectra of linear and cyclized DNHB peptides.

Table S1. Chemical shift difference of diasteretopic Hα protons of Gly7 and the root mean square deviation (RMSD) of ΔδHα values for the cyclized peptides.

Peptide	Gly splitting (ppm)	RMSD
DNHB 1.1	0.20 (±0.02)	0.17 (±0.04)
DNHB 1.2	0.20 (±0.02)	0.15 (±0.02)
DNHB 1.3	0.29 (±0.02)	0.27 (±0.05)
DNHB 2.1	0.25 (±0.03)	0.14 (±0.05)
DNHB 2.2	0.48 (±0.02)	0.38 (±0.03)
DNHB 2.3	0.43 (±0.03)	0.35 (±0.02)
DNHB 3.1	0.33 (±0.04)	0.28 (±0.03)
DNHB 3.2	0.45 (±0.02)	0.41 (±0.07)
DNHB 3.3	0.46 (±0.03)	0.41 (±0.05)

Table S2. : Nonsequential NOEs contacts involving backbone protons of cyclic DNHB 2.2 peptide.

Residue	Proton	Proton	Residue
Hpg^{2}	HA	HN	Lys^{12}
Thr^{3}	HN	HA	Val^{11}
Thr^{3}	HN	HN	Thr^{10}
Trp^{4}	HA	HN	Thr^{10}
Trp^{4}	HA	HA	Dab^{9}
Glu^{5}	HN	Hα	Dab^{9}
Glu^{5}	HN	HN	Lys^{8}

Table S3: Temperature dependence of the amide protons for cyclic DNHB 2.2 peptide.

Residue	Δδ (ppb)/ΔT (K)
Ser1	-9.8
Hpg2	-9
Thr3	-3.9
Trp4	-11
Glu5	-4.1
Asn6	-9.8
Gly7	-8.7
Lys8	-3.8
Dab9	-11
Thr10	-4.5
Val11	-9
Lys12	-4.6

Table S4. : Nonsequential NOEs contacts involving backbone protons of cyclic DNHB 2.2W3 peptide.

Residue	**Proton**	**Proton**	**Residue**
Trp^{3}	HN	HA	Val^{11}
Trp^{3}	HN	HN	Thr^{10}
Thr^{4}	HA	HN	Thr^{10}
Glu^{5}	HN	HN	Lys^{8}