

Supporting Information

α,ϵ -Hybrid Peptide Foldamers: Self-assembly of Peptide with *trans* Carbon-Carbon Double Bonds in the Backbone and its Saturated Analogue

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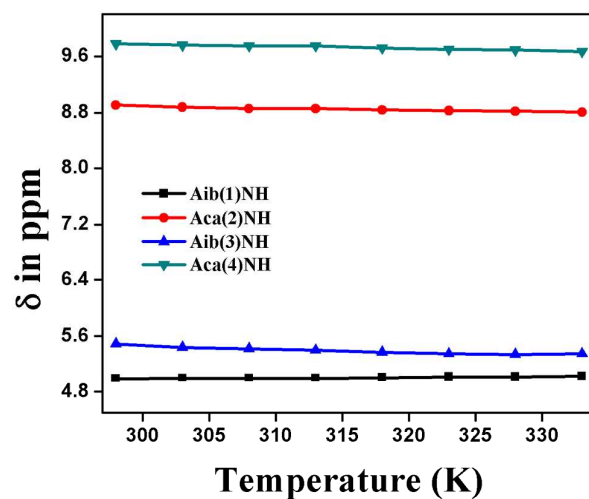


Figure S1: Plot of temperature dependence of NHs chemical shifts of Peptide 1 in CDCl_3 solution.

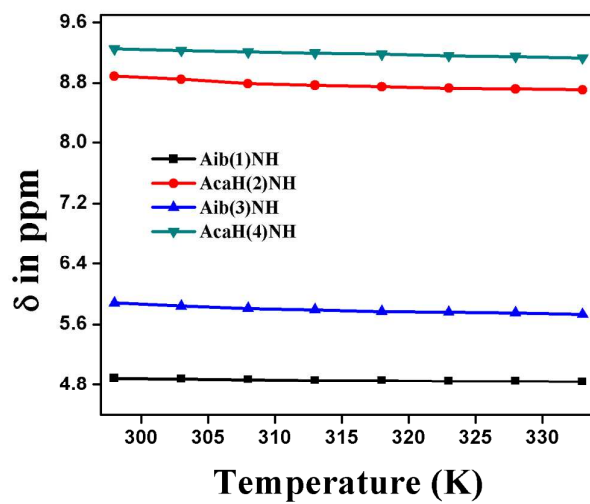


Figure S2: Plot of temperature dependence of NHs chemical shifts of Peptide 2 in CDCl_3 solution.

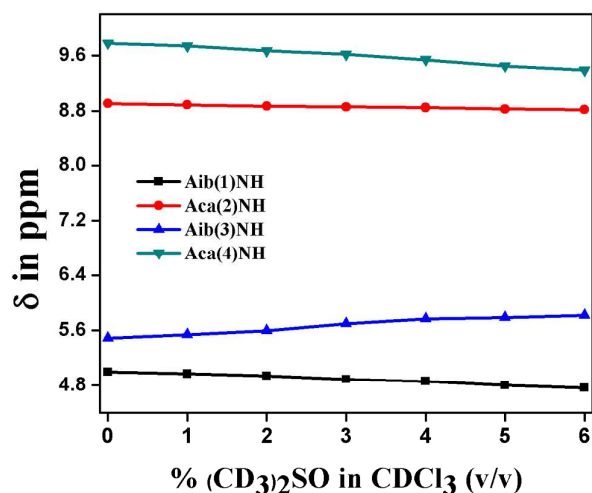


Figure S3: Plot of solvent dependence of NHs chemical shifts of peptide **1** at varying concentrations of (CD₃)₂SO in CDCl₃ solution.

Table S1: Characteristic ¹H NMR parameters for peptide **1** (chemical shifts δ)^a

Residue	δ (NH)	$\Delta\delta^b$	$\Delta\delta^c$
Aib(1)NH	4.99	-0.23	0.04
Aca(2)NH	8.91	-0.09	-0.10
Aib(3)NH	5.49	0.33	-0.17
Aca(4)NH	9.78	-0.39	-0.11

^a Chemical shift values of NH proton resonances for peptide **1** in CDCl₃.

^b $\Delta\delta$ is the chemical shift difference for NH protons in CDCl₃ and 6% (CD₃)₂SO/CDCl₃ for peptide **1**.

^c $\Delta\delta$ is the chemical shift difference for NH protons in CDCl₃ on heating from 298 K to 333 K for peptide **1**.

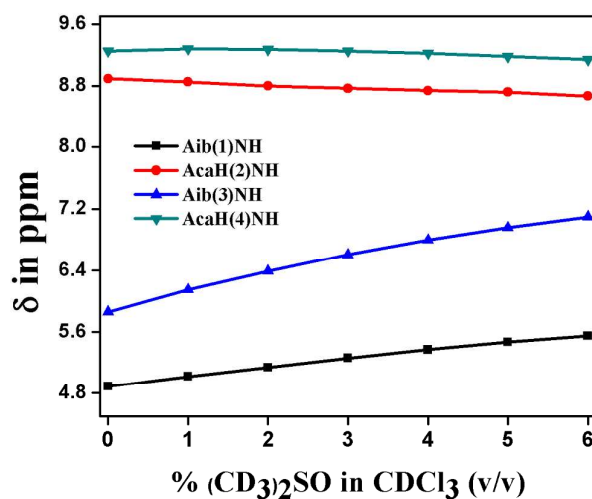


Figure S4: Plot of solvent dependence of NHs chemical shifts of peptide **2** at varying concentrations of (CD₃)₂SO in CDCl₃ solution.

Table S2: Characteristic ^1H NMR parameters for peptide **2** (chemical shifts δ)^a

Residue	δ (NH)	$\Delta\delta^b$	$\Delta\delta^c$
Aib(1)NH	4.89	0.66	-0.05
AcaH(2)NH	8.89	-0.22	-0.18
Aib(3)NH	5.88	1.24	-0.15
AcaH(4)NH	9.25	-0.11	-0.12

^a Chemical shift values of NH proton resonances for peptide **2** in CDCl_3 .

^b $\Delta\delta$ is the chemical shift difference for NH protons in CDCl_3 and 6% $(\text{CD}_3)_2\text{SO}/\text{CDCl}_3$ for peptide **2**.

^c $\Delta\delta$ is the chemical shift difference for NH protons in CDCl_3 on heating from 298 K to 333 K for peptide **2**.

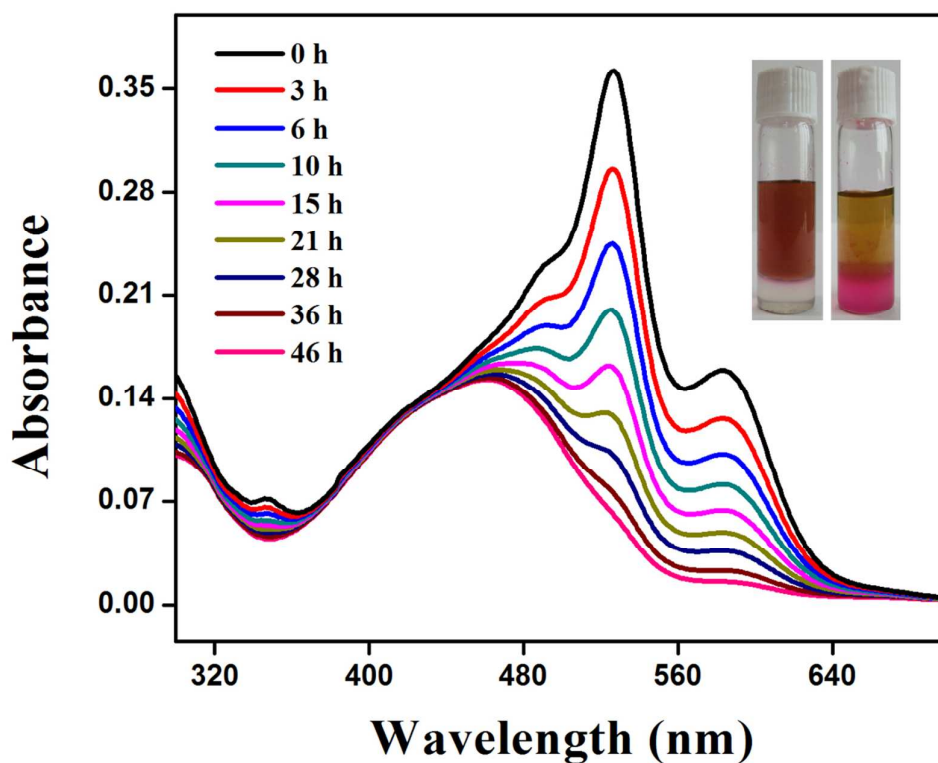


Figure S5: Removal of cationic dyes (rhodamine 6G and methyl violet) selectively from waste water (a mixture of rhodamine 6G, methyl violet, methyl orange and pyrocatechol violet) using peptide **2** gel from xylene.

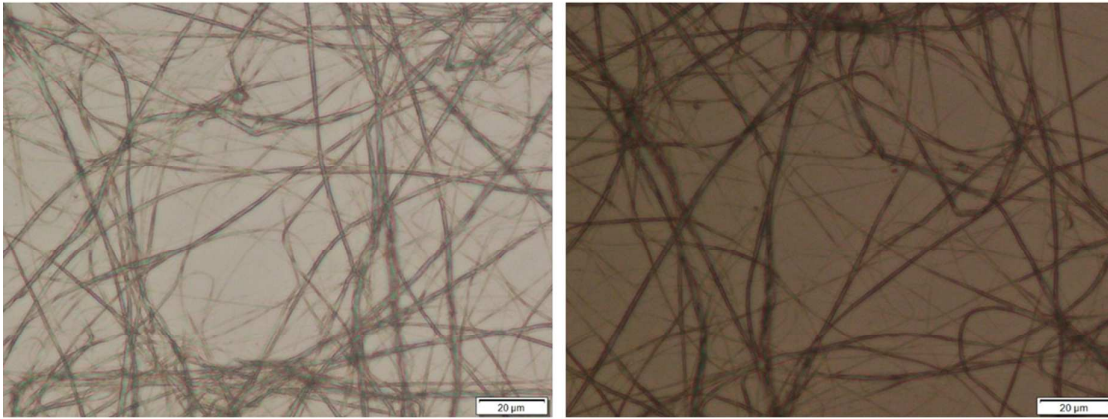


Figure S6: The POM images of peptide **2** xerogel showing fibrous network.

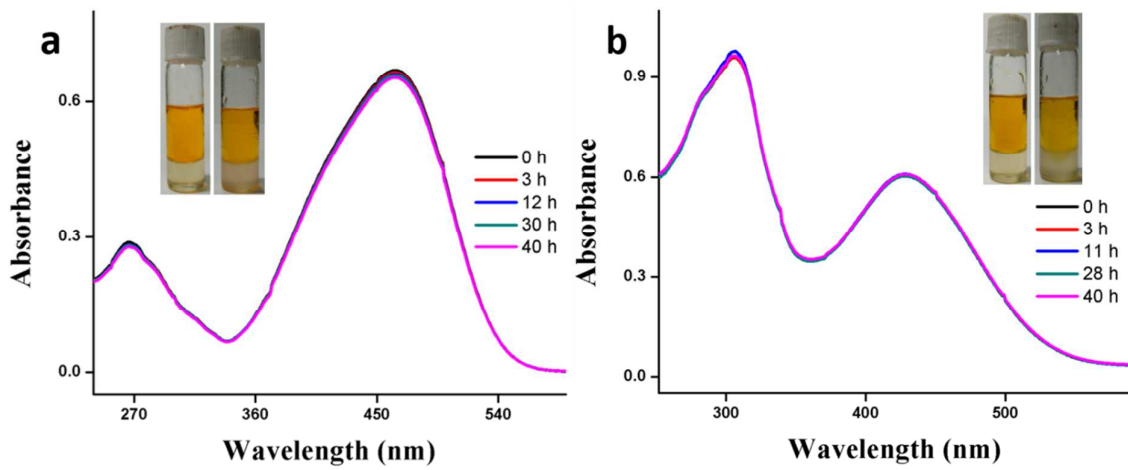


Figure S7: Dye removal studies using peptide **2** gel from xylene showing no absorption; (a) Methyl orange (anionic) and (b) pyrocatechol violet (neutral).

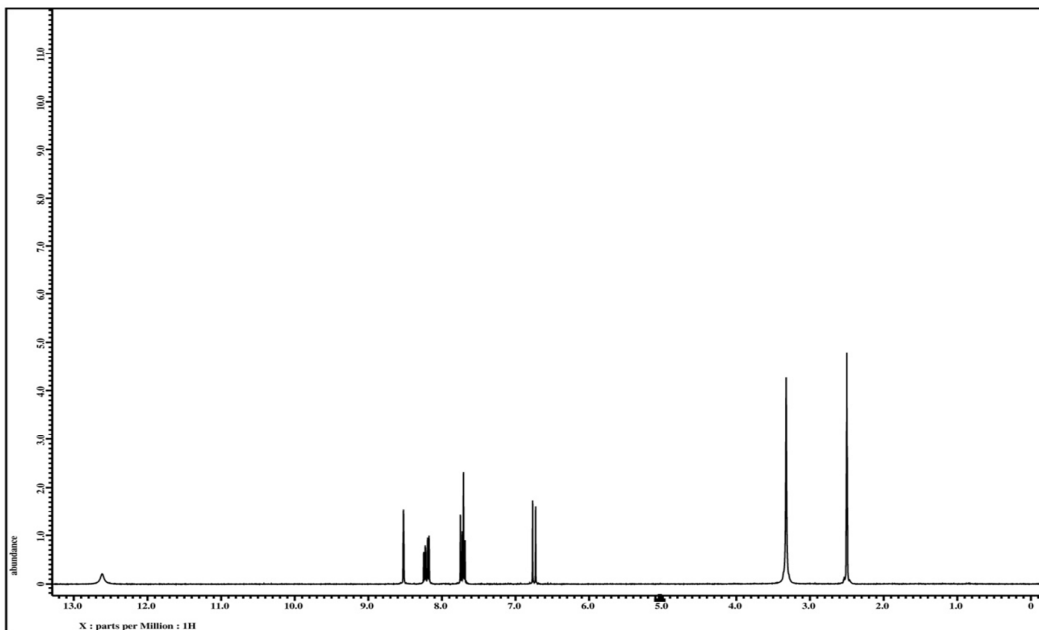


Figure S8: ¹H NMR (400 MHz, DMSO-*d*₆, δppm) spectrum of *trans*-3-Nitrocinnamic acid 4.

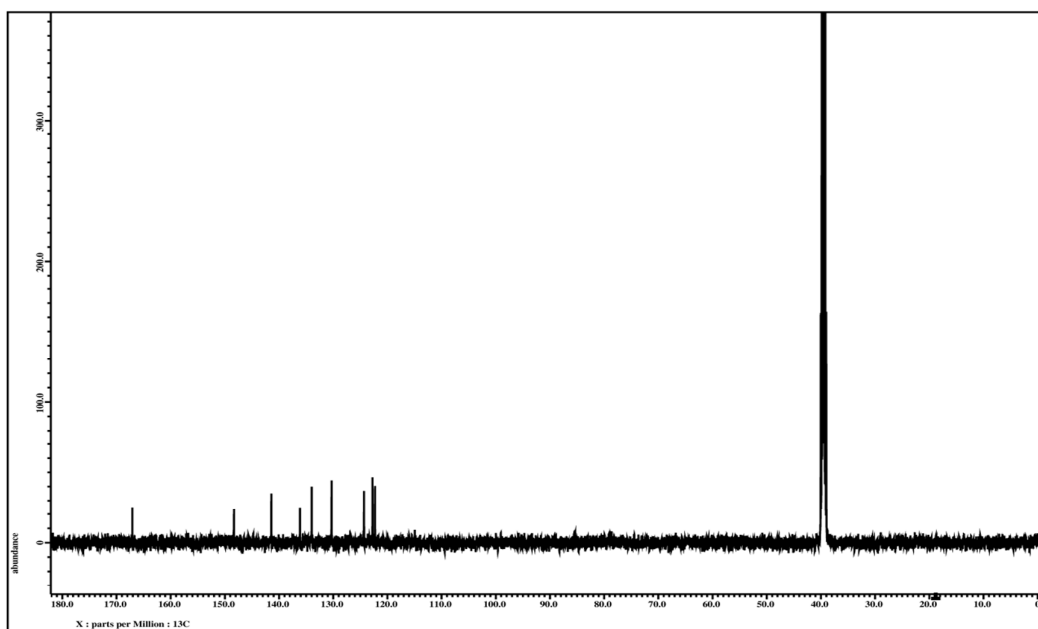


Figure S9: ¹³C NMR (125 MHz, DMSO-*d*₆, δppm) spectrum of *trans*-3-Nitrocinnamic acid 4.

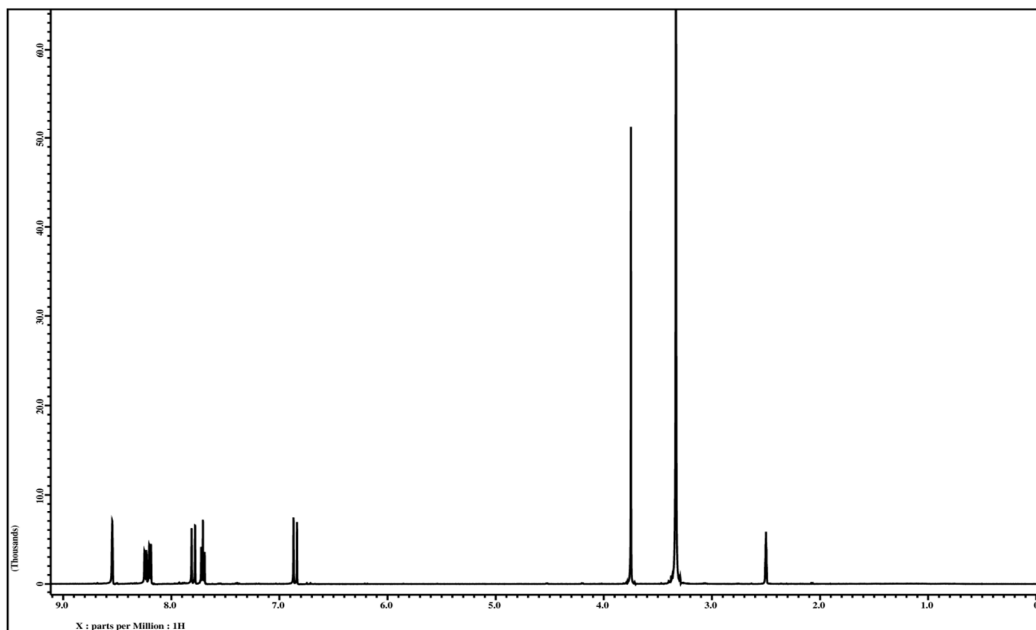


Figure S10: ¹H NMR (500 MHz, DMSO-*d*₆, δppm) spectrum of **Methyl (E)-3-nitrocinnamate 5**.

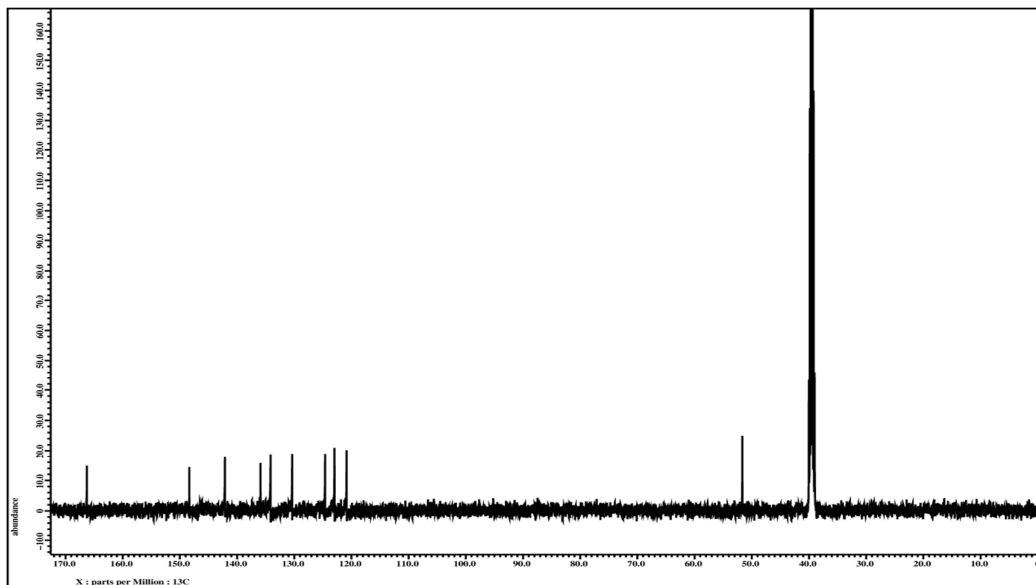


Figure S11: ¹³C NMR (125 MHz, DMSO-*d*₆, δppm) spectrum of **Methyl (E)-3-nitrocinnamate 5**.

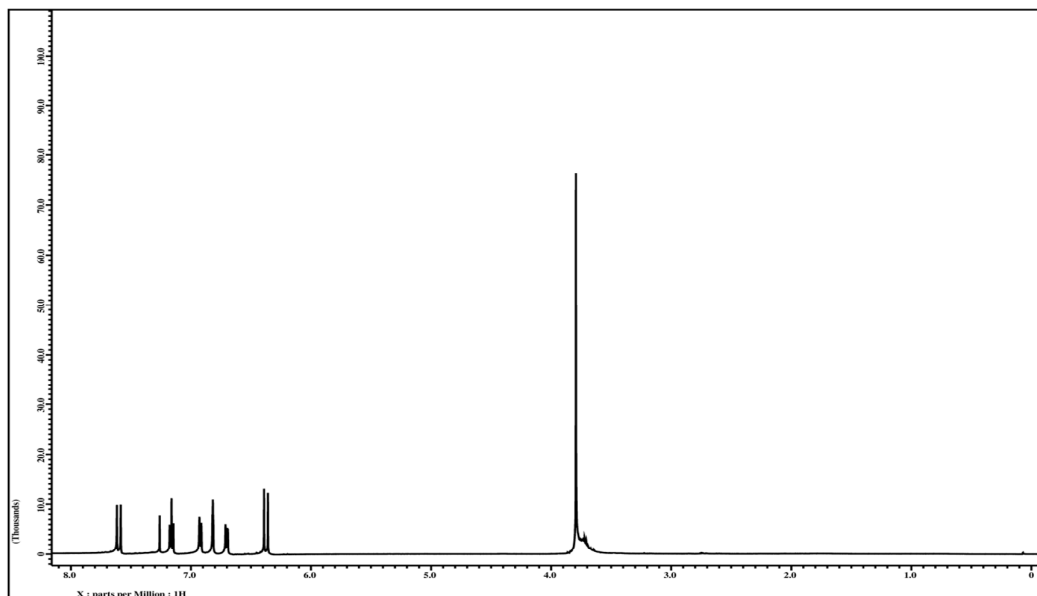


Figure S12: ¹H NMR (500 MHz, CDCl₃, δppm) spectrum of **Methyl (E)-3-aminocinnamate 6**.

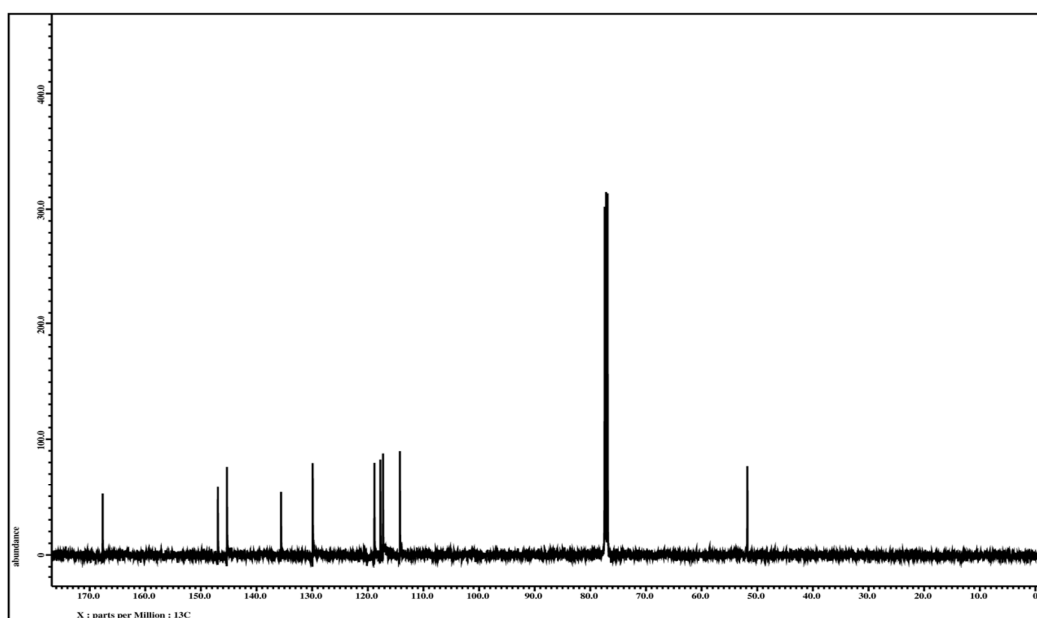


Figure S13: ¹³C NMR (125 MHz, CDCl₃, δppm) spectrum of **Methyl (E)-3-aminocinnamate 6**.

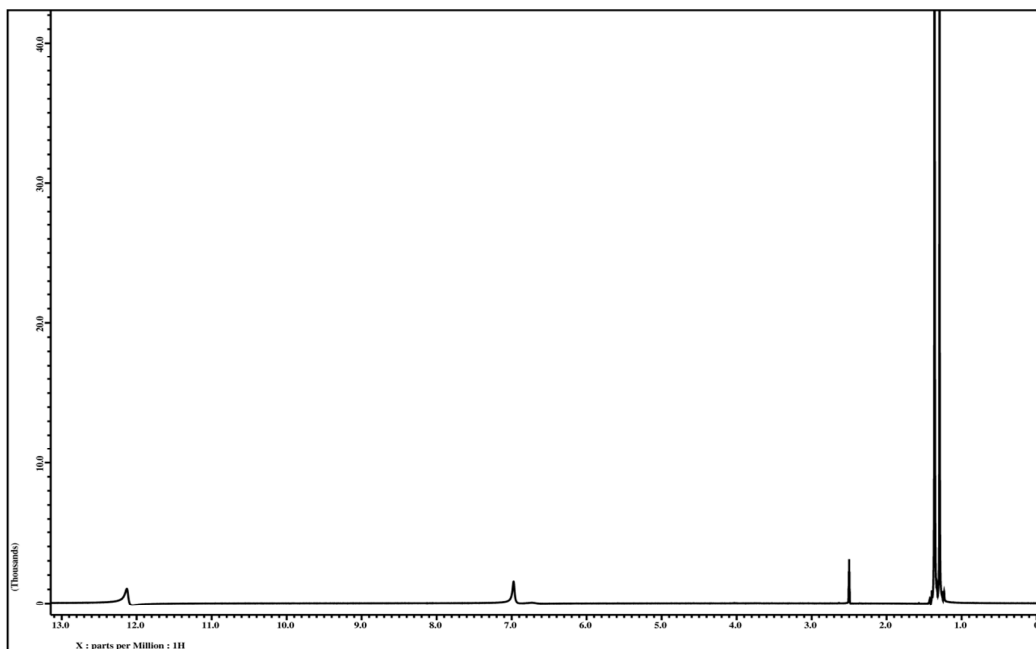


Figure S14: ^1H NMR (500 MHz, $\text{DMSO-}d_6$, δppm) spectrum of **Boc-Aib-OH 7**.

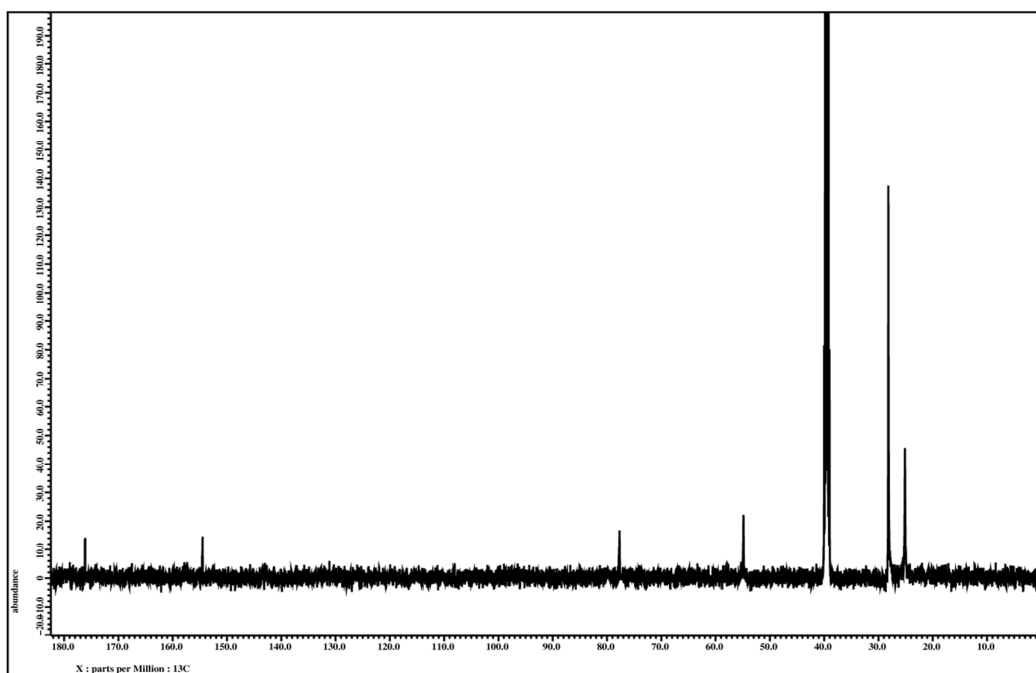


Figure S15: ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$, δppm) spectrum of **Boc-Aib-OH 7**.

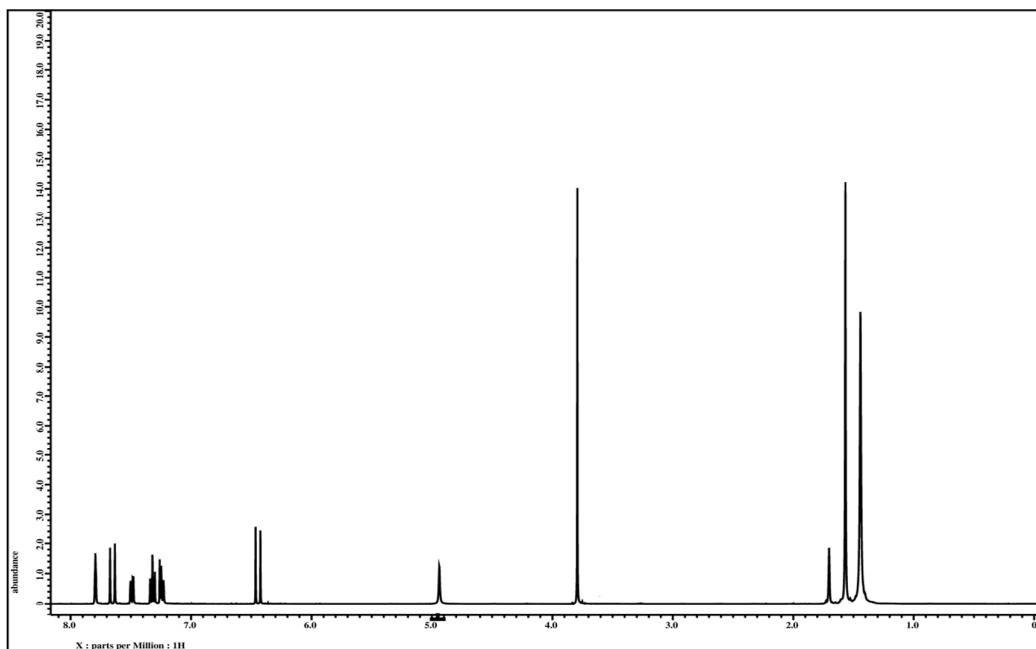


Figure S16: ¹H NMR (400 MHz, CDCl₃, δppm) spectrum of **8**.

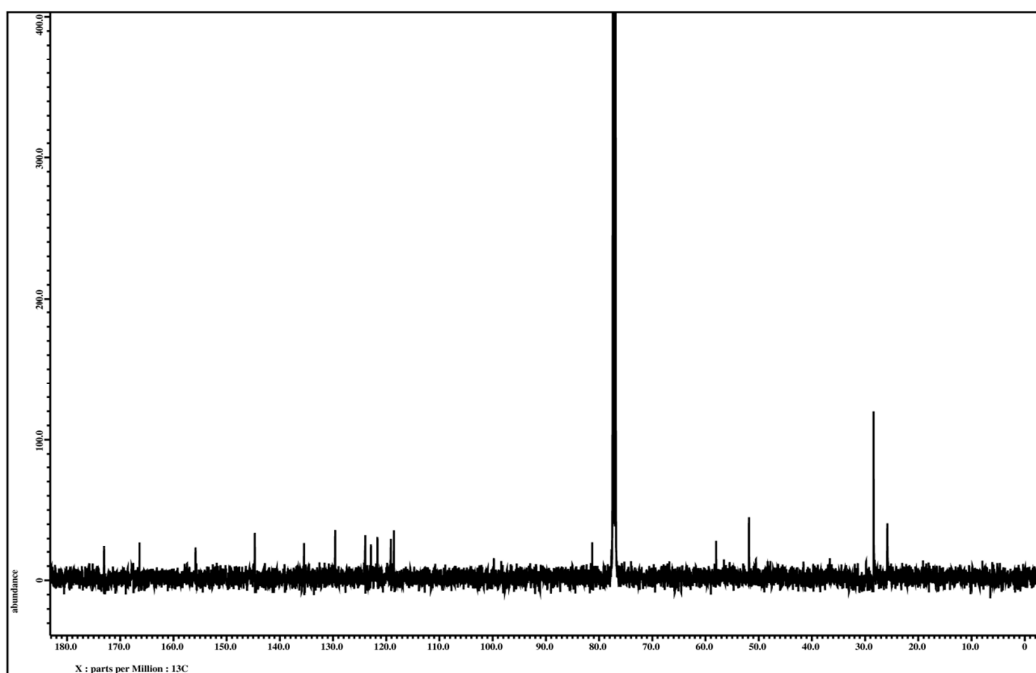


Figure S17: ¹³C NMR (125 MHz, CDCl₃, δppm) spectrum of **8**.

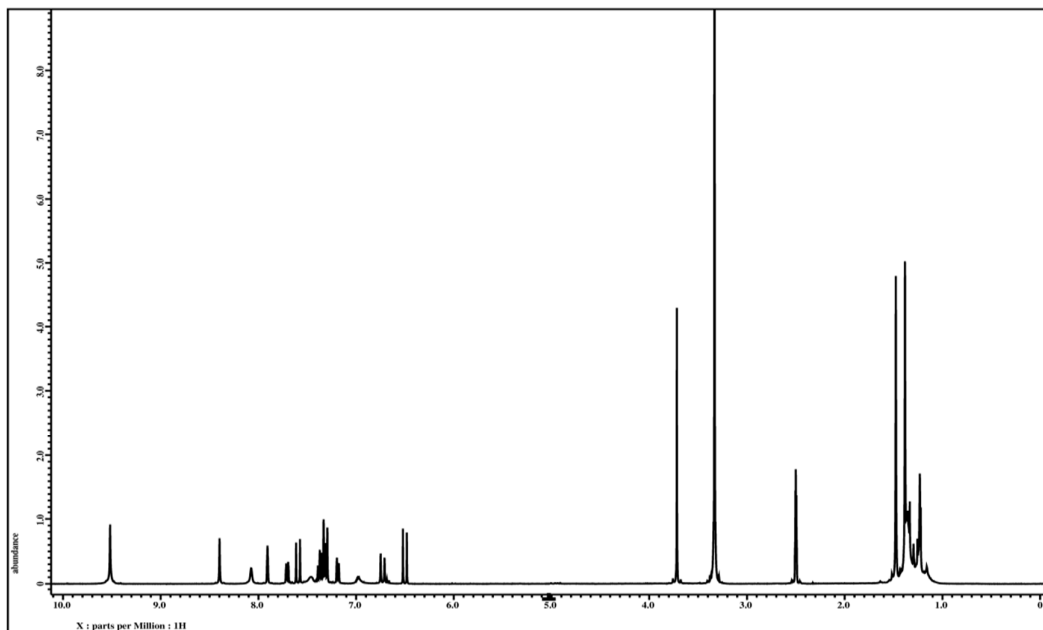


Figure S18: ^1H NMR (400 MHz, $\text{DMSO-}d_6$, δppm) spectrum of **1**.

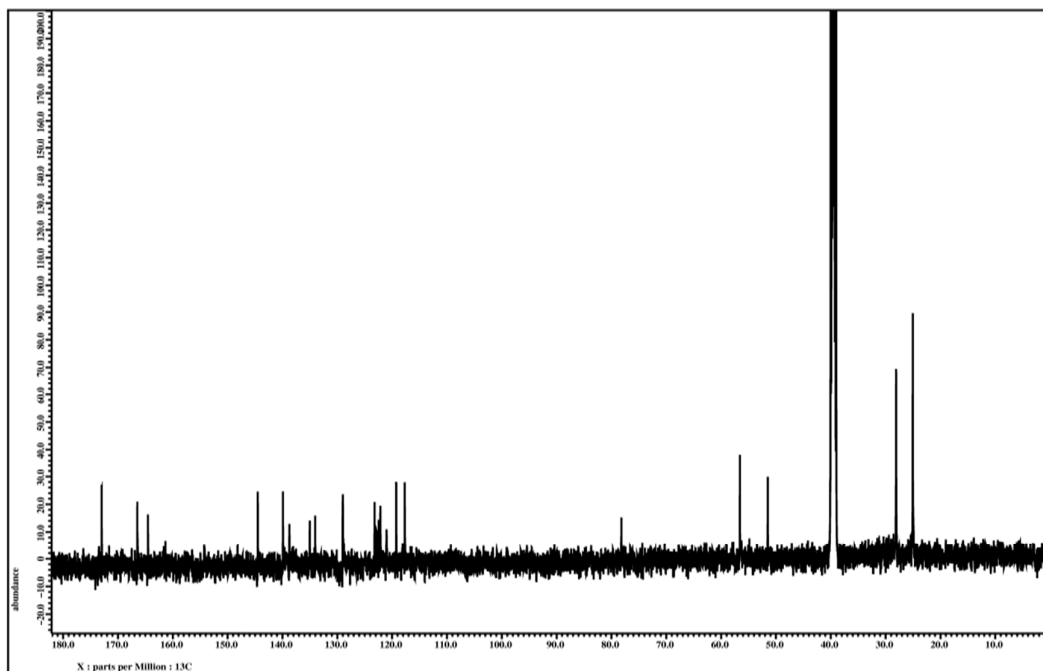


Figure S19: ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$, δppm) spectrum of **1**.

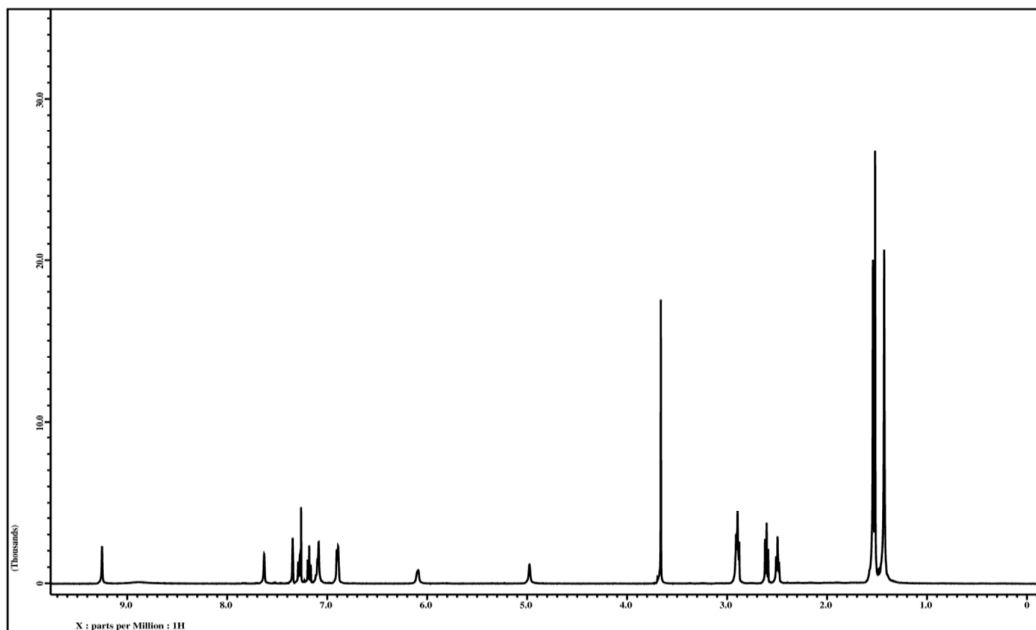


Figure S20: ^1H NMR (500 MHz, CDCl_3 , δppm) spectrum of **2**.

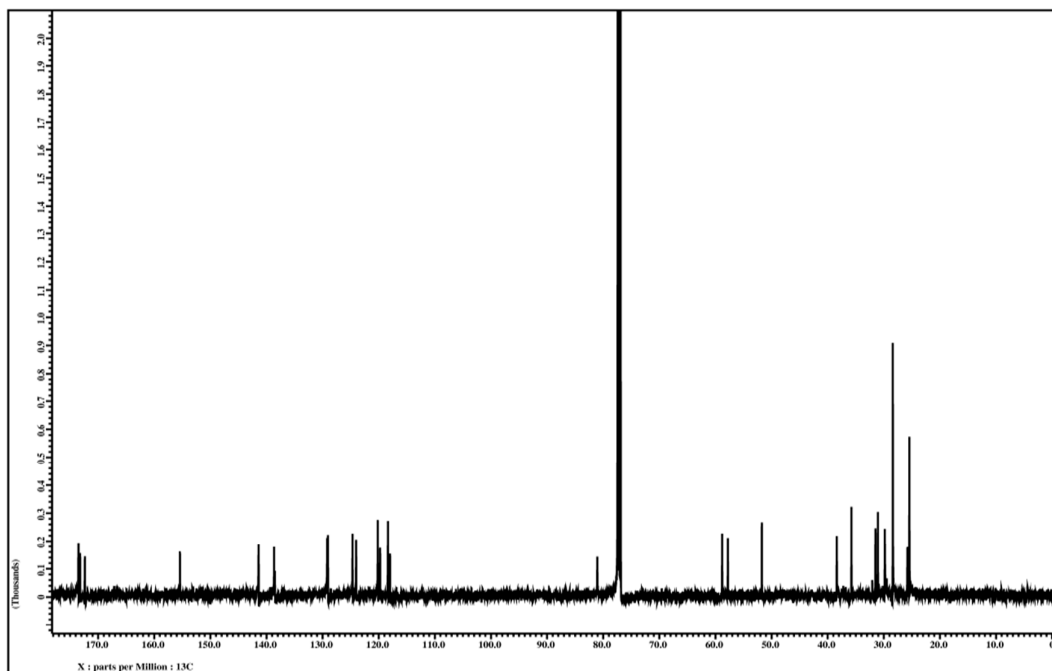


Figure S21: ^{13}C NMR (125 MHz, CDCl_3 , δppm) spectrum of **2**.

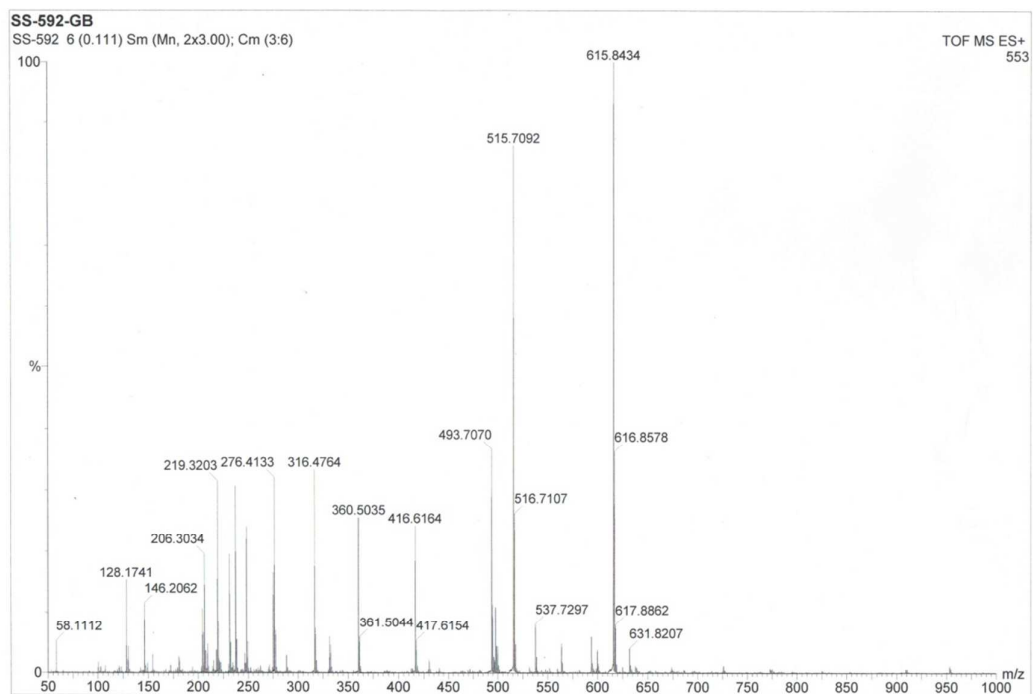


Figure S22: Mass spectrum of peptide 1.

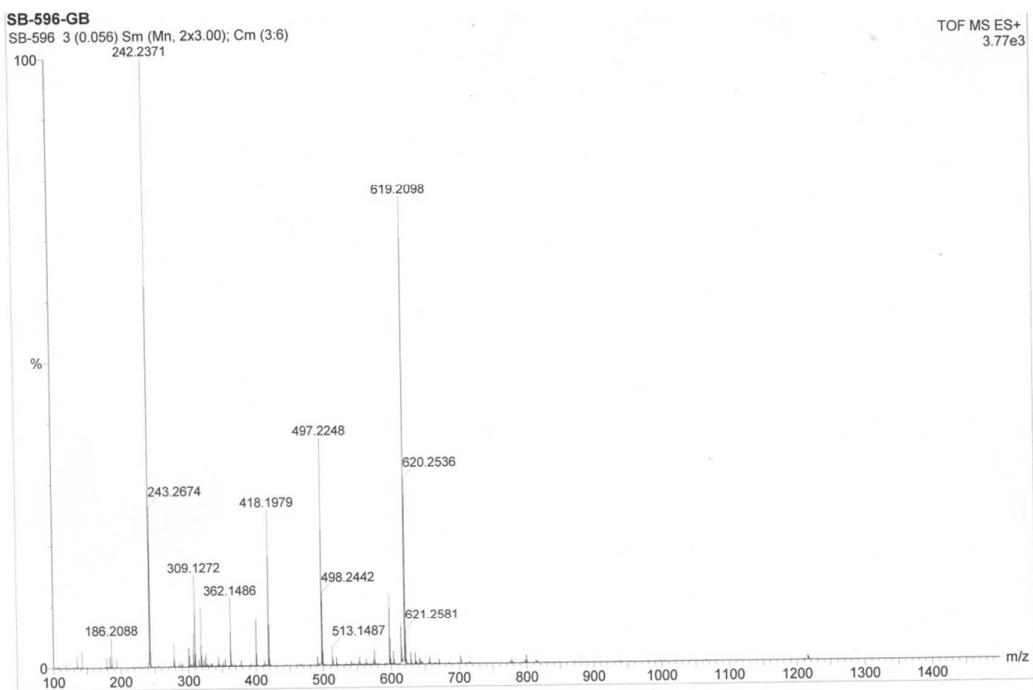


Figure S23: Mass spectrum of peptide 2.

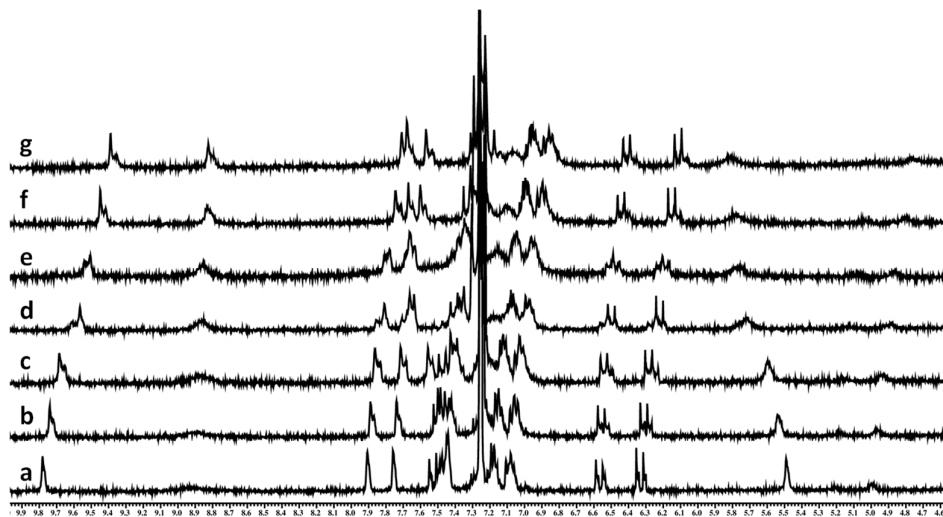


Figure S24: Part of ¹H NMR (400 MHz) solvent titration spectra of peptide **1** in CDCl₃ solution. % of DMSO-d₆ a) 0, b) 1, c) 2, d) 3, e) 4, f) 5 and g) 6.

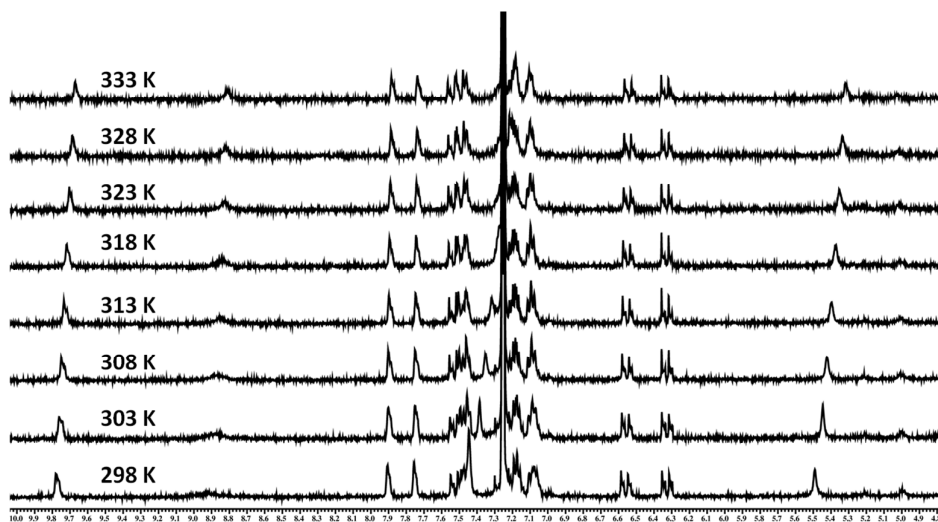


Figure S25: Part of ¹H NMR (400 MHz) spectra of peptide **1** at variable temperature in CDCl₃.

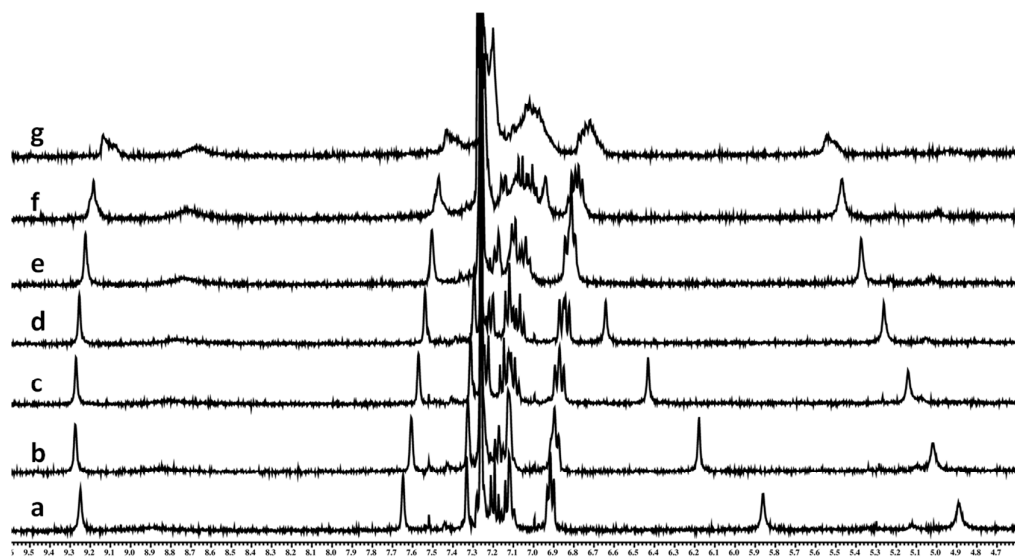


Figure S26: Part of ¹H NMR (400 MHz) solvent titration spectra of peptide **2** in CDCl₃ solution. % of DMSO-d₆ a) 0, b) 1, c) 2, d) 3, e) 4, f) 5 and g) 6.

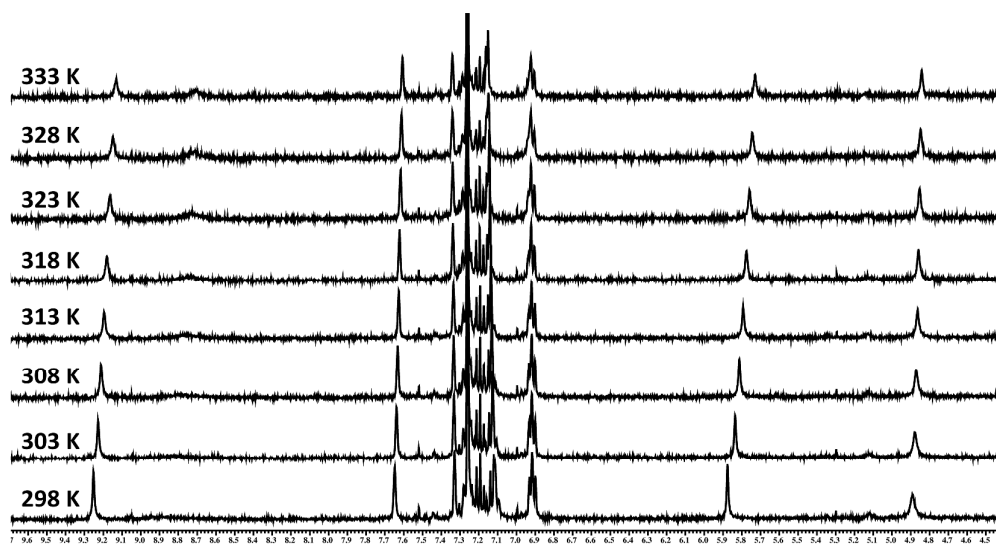


Figure S27: Part of ¹H NMR (400 MHz) spectra of peptide **2** at variable temperature in CDCl₃.