Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Effect of spacer on the structure and self-assembly of FF peptide mimetic†

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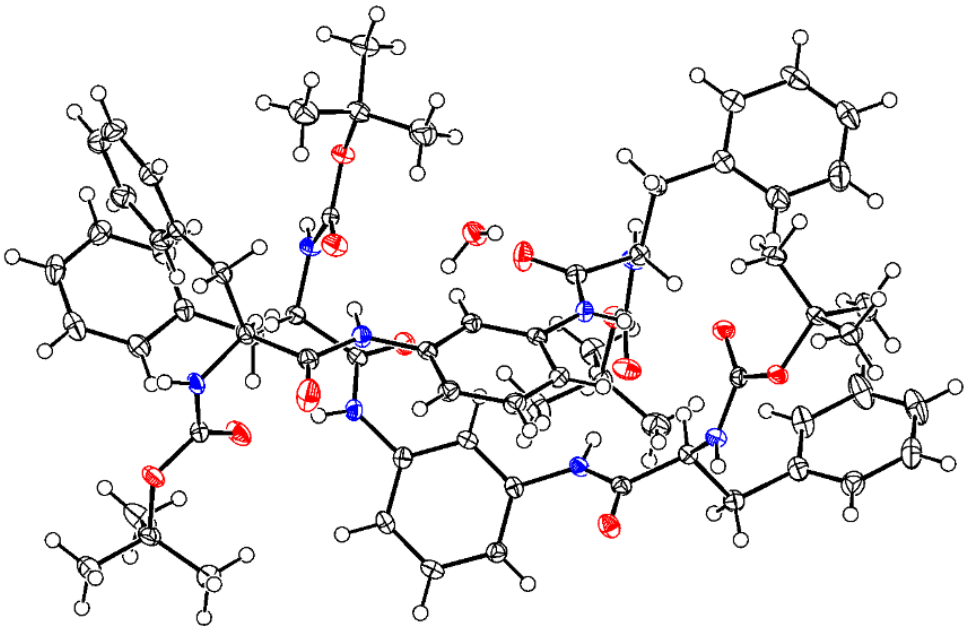

Fig. S1: The ORTEP diagram of FF peptide mimetics **3**. 50% probability.

	Peptide 3
Space group	*P21*
Crystal system	Monoclinic
a **(Å)**	10.85569 (8)
b **(Å)**	25.04851 (19)
c **(Å)**	12.39611 (9)
α **(°)**	90
β (°)	99.6153 (7)
γ (°)	90
Volume (Å^3)	3323.38 (4)
Temperature (K)	293
Z/Z'	2
D_{calc} **(Mg/m^3)**	1.223
θ_{min}-θ_{max} **(°)**	3.5, 68.3
Total reflections/unique/R_{int}	30376, 12152, 0.033
Observed data(I>2 σ(*I*))	9514
Nref/Npar	9643, 821
R_1/wR_2 **(all data)**	0.0269, 0.06979

Table S1: Data collection and refinement statistic for peptide **3**

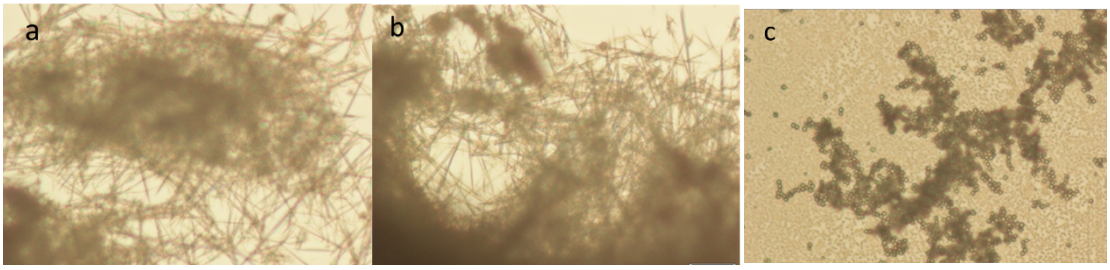

Fig. S2: (a) The POM image of the FF peptide mimetic 1 xerogel in methanol. (b) The POM image of the FF peptide mimetic 2 xerogel from methanol showing entangled fibers like morphology. (c) The POM image of the FF peptide mimetic 3 in methanol solution showing polydisperse microsphere morphology.

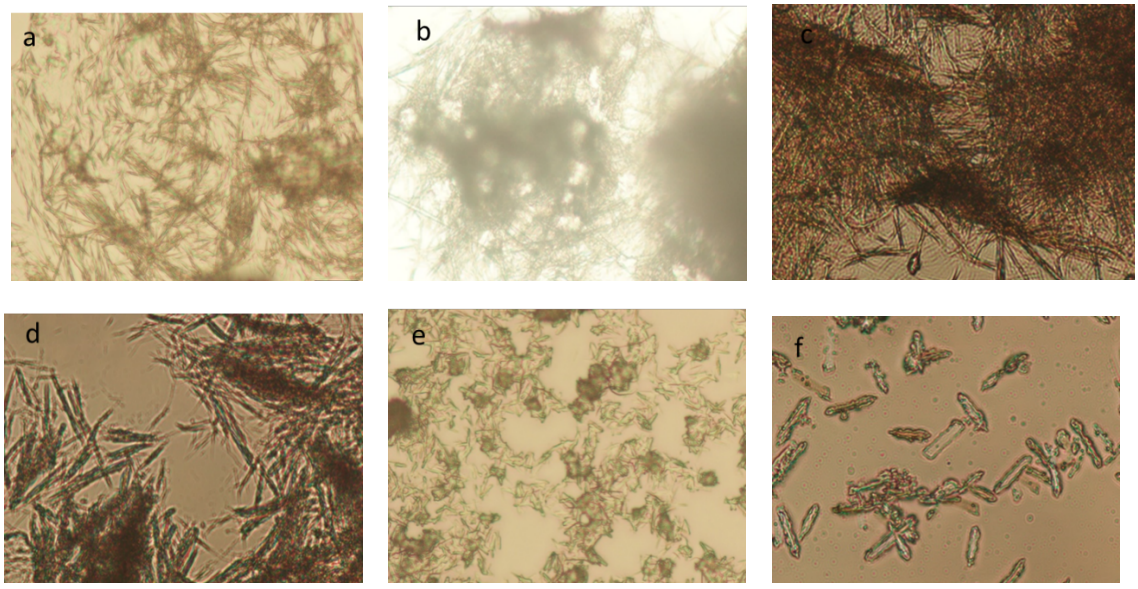

Fig. S3: The POM images of FF peptide mimetic **1** xerogel from (a) benzene and (b) chlorobenzene. The POM images of FF peptide mimetic **2** xerogel from (c) benzene and (d) chlorobenzene. The POM images of FF peptide mimetic **3** from (e) benzene solution and (f) chlorobenzene solution.

Synthesis

Boc-Phenylalanine

L-Phenylalanine 1.6519 g (10 mmol) was dissolved in a mixture of dioxane (20 ml), water (10 ml) and 1 M NaOH (20 ml), stirred and cooled in ice water, Di-tert-bupyrodicarbonate 2.619 g (12 mmol) was added and stirred for 6 hrs at room temperature. The solution was concentrated using rotary evaporator to about 20 – 25 ml. Cooled down and Ethyl acetate (30 ml) was added, acidified with dilute solution of $KHSO_4$ (saturated solution) to pH 2-3 (cungo red). The compound was extracted with Ethyl acetate three times. Dry with Na2SO4 and evaporated under vacuum. The pure material Boc-Phenylalanine was obtained as waxy solid.

Yield: 93.12%

^{1}H NMR (DMSO-d_6, 500 MHz, δppm): 12.75 (br, 1H, COOH); 7.28- 7.09 (m, 5H, aromatic ring protons); 7.11-7.09 (d, 1H, J = 10Hz, Phe NH); 4.09-4.01 (m, 1H, C$^{\alpha}$H Phe); 3.02-2.87 (m, 2H, C$^{\beta}$H Phe), 1.36 (s, 9H, Boc -CH_3). ^{13}C NMR (DMSO-d_6, 125 MHz, δ in ppm, 298K): 173.57, 155.41, 138.00, 129.05, 128.09, 126.27, 80.24, 55.10, 36.39, 20.73.

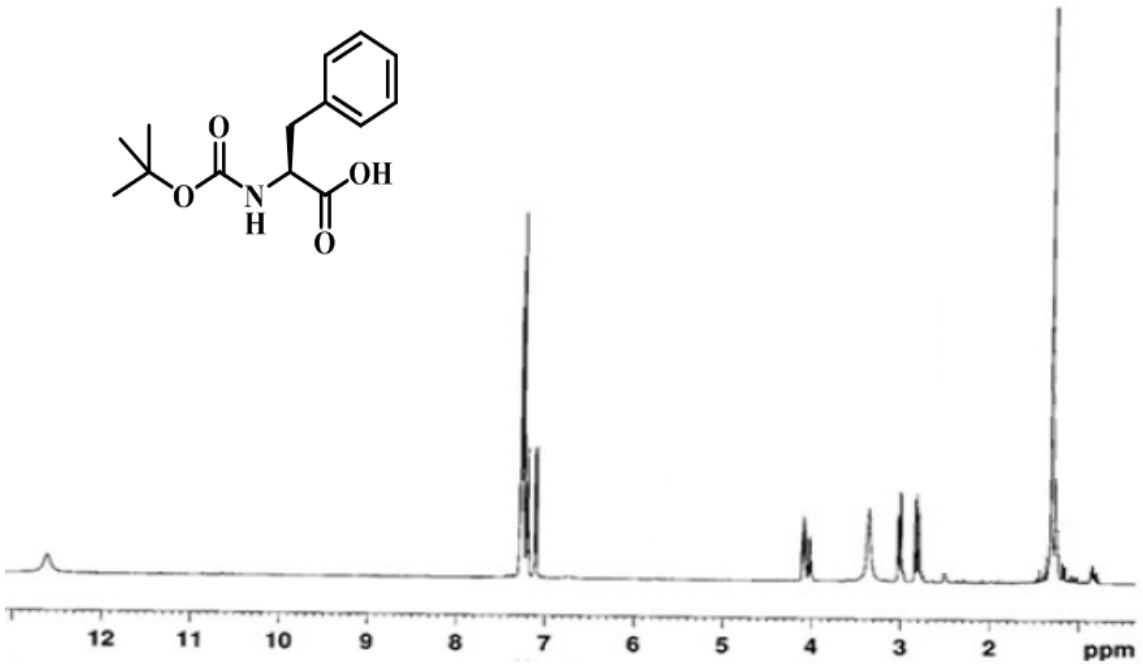

Fig. S4: ^{1}H NMR (500 MHz, DMSO-d_6, δ in ppm, 298K) spectrum of Boc-Phe-OH.

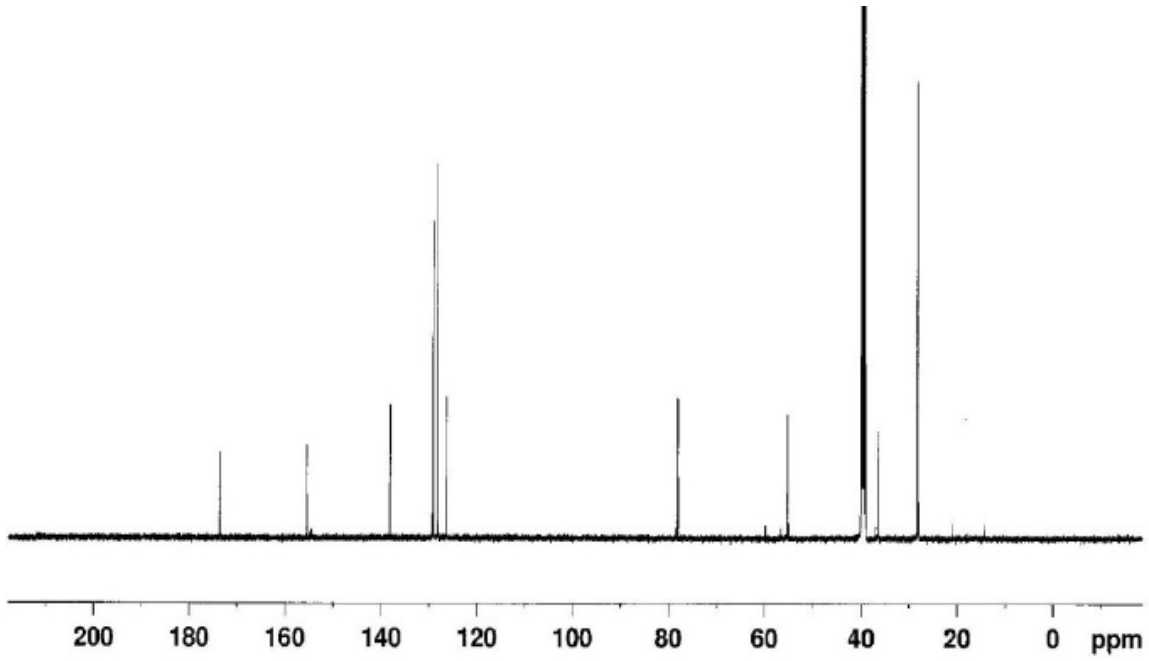

Fig. S5: ^{13}C NMR (125 MHz DMSO-d_6, δ in ppm, 298K) spectrum of Boc-Phe-OH.

Peptide mimetic **1**

Boc-phenylalanine 2.653 g (10 mmol) was dissolved in 20 mL of dry DCM and 5 ml of dry DMF under ice−water bath conditions, followed by the addition of 3.095 g (15 mmol) of DCC and 2.297 g (15 mmol) of HOBt. 0.441 g (5 mmol) 1,4-diaminobutane was then added to the solution. The reaction mixture was stirred for 48 h at room temperature. After the completion of the reaction, DCM was evaporated, and the residue was dissolved in ethyl acetate (40 mL) and was put in fridge for 3 h for dicyclohexylurea (DCU) to precipitate, dicyclohexylurea (DCU) was filtered off and water (50 ml) was added and stirred at room temperature for 30 min and subsequently, the ethyl acetate layer was washed with 2 M HCl (3 × 50 mL), brine (2 × 50 mL), 1 M sodium carbonate (3 × 50 mL), and brine (2 × 50 mL), respectively. The organic layer was dried over anhydrous sodium sulfate and evaporated under vacuum to yield peptide **1** as waxy solid. The product was purified by silica gel using hexane/ethyl acetate (4/1) as eluent. Yield: 97 %.

^1H NMR (DMSO-d_6, 500MHz, δppm): 7.82 (s, 2H, butene NH), 7.18-7.25 (m, 10H, Phenyl ring protons), 6.82-6.84 (s, 2H, Phe NH), 4.12 (m, 2H, Phe $C^{\alpha}H$), 3.03 (d, 4H, butene CH), 2.80-2.95 (m, 4H, Phe $C^{\beta}H$), 1.29 (s, 18H, BOC -CH_3), 1.22 (d, 4H, butene CH). ^{13}C NMR (125MHz, DMSO-d_6, δ in ppm, 298K): 172.14, 154.43, 138.20, 136.16, 129.15, 127.94, 126.12, 77.88, 56.46, 39.93, 38.89, 28.12, 26.13; ESI-MS (MeOH): m/z (Calc): $C_{32}H_{46}N_4O_6Na$ 606.33; found: 606.36.

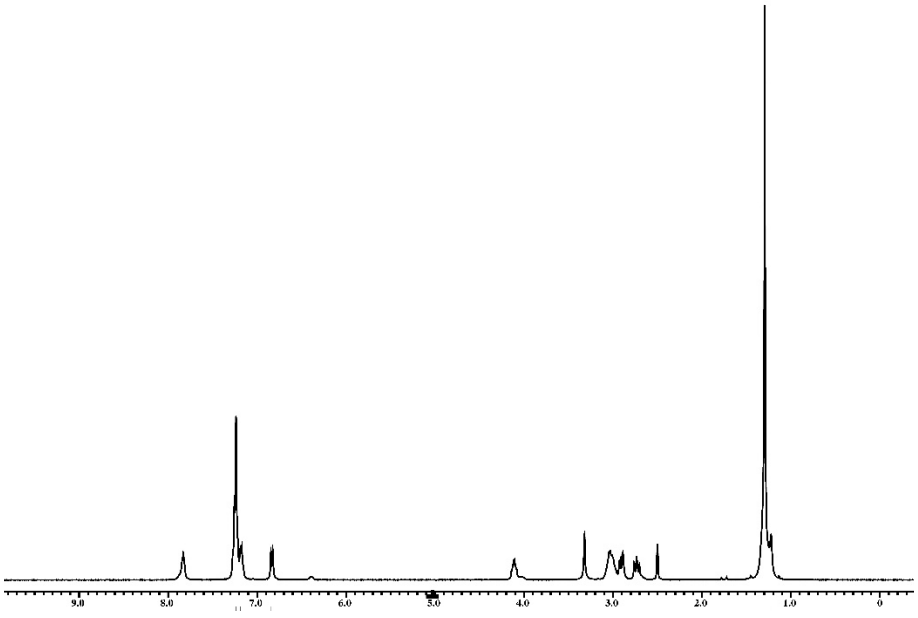

Fig. S6: ^{1}H NMR (400 MHz, DMSO-d_6, δ in ppm, 298K) spectrum of peptide mimetic **1**

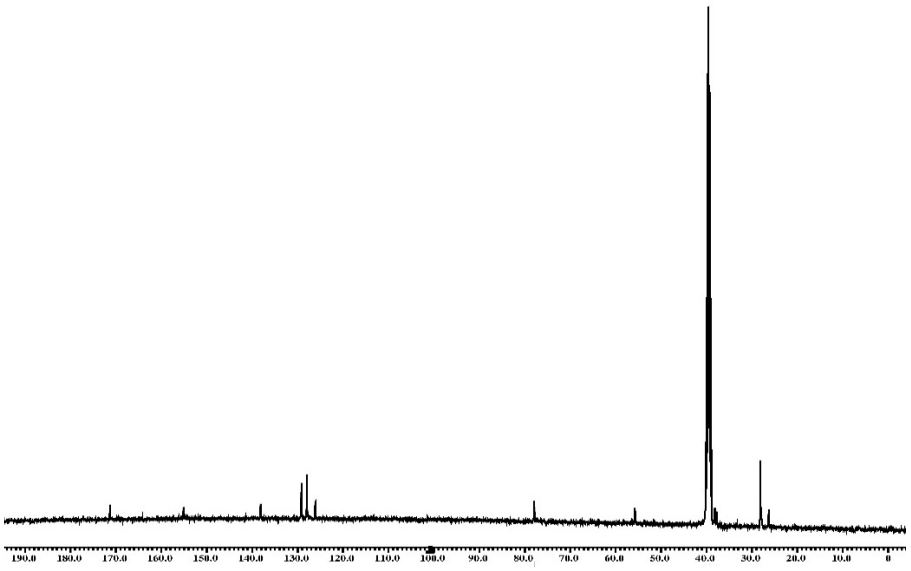

Fig. S7: ^{13}C NMR (100 MHz, DMSO-d_6, δ in ppm, 298K) spectrum of peptide mimetic **1**

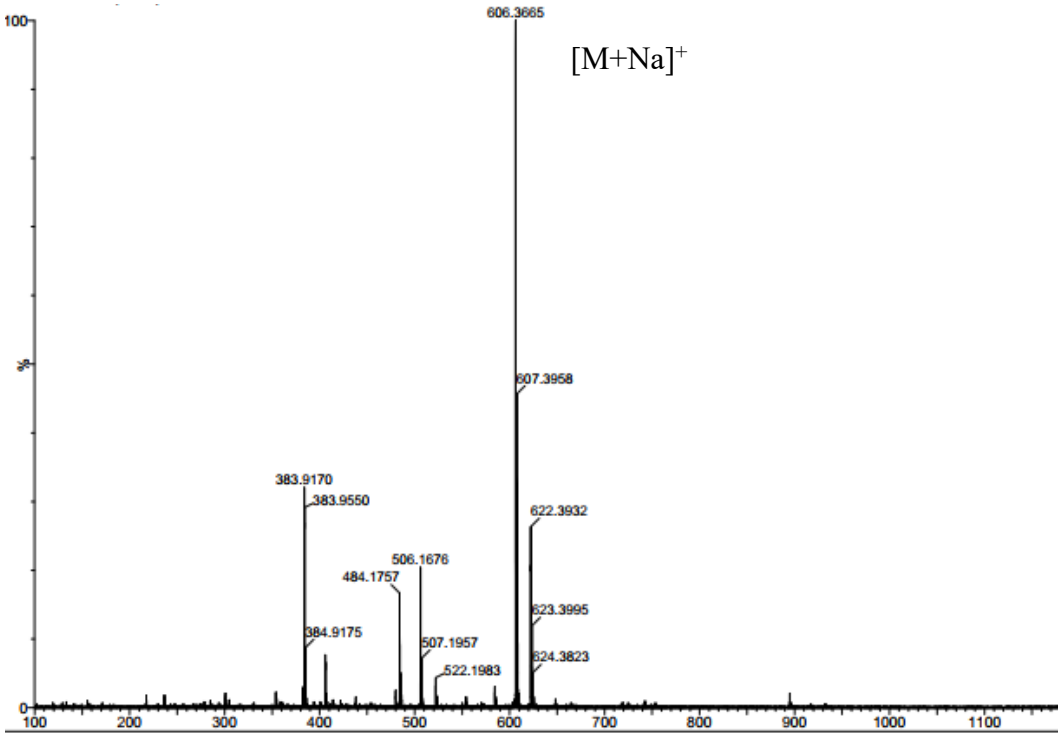

Fig. S8: Mass Spectrum of peptide mimetic **1**

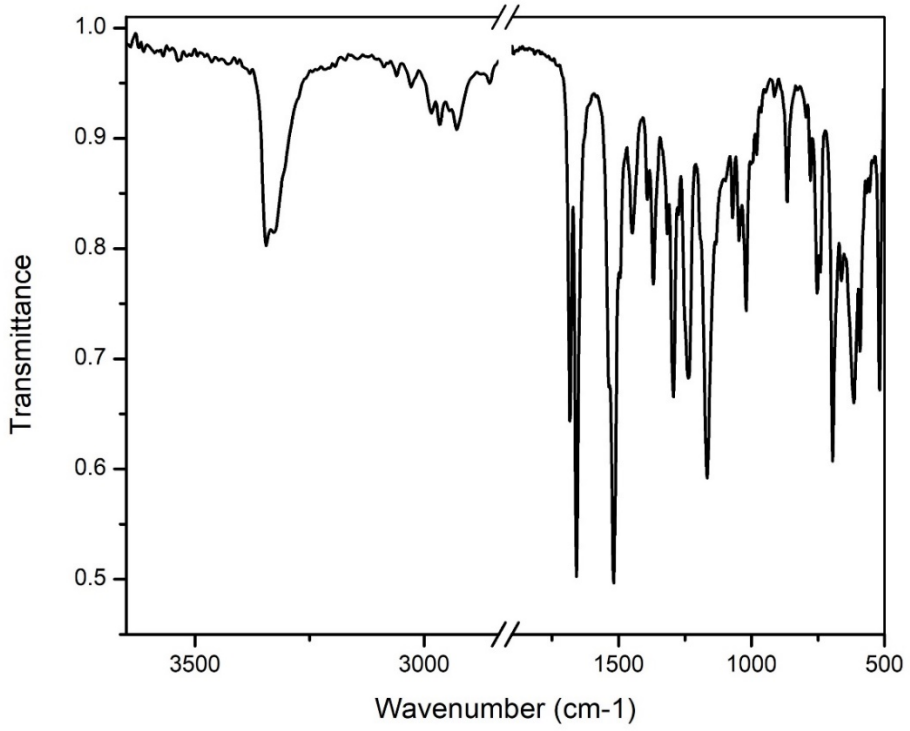

Fig. S9: FT-IR Spectrum of peptide mimetic **1**

Peptide mimetic **2**

Boc-phenylalanine 2.653 g (10 mmol) was dissolved in 20 mL of dry DCM and 5 ml of dry DMF under ice–water bath conditions, followed by the addition of 3.095 g (15 mmol) of DCC and 2.297 g (15 mmol) of HOBt. 0.613 g (4.5 mmol) m-xylenedine diamine was then added to the solution. The reaction mixture was stirred for 48 h at room temperature. After the completion of the reaction, DCM was evaporated, and the residue was dissolved in ethyl acetate (40 mL) and was put in fridge for 3 h for dicyclohexylurea (DCU) to precipitate, dicyclohexylurea (DCU) was filtered off and water (50 ml) was added and stirred at room temperature for 30 min and subsequently, the ethyl acetate layer was washed with 2 M HCl (3 × 50 mL), brine (2 × 50 mL), 1 M sodium carbonate (3 × 50 mL), and brine (2 × 50 mL), respectively. The organic layer was dried over anhydrous sodium sulfate and evaporated under vacuum to yield peptide **2** aswaxy solid. The product was purified by silica gel using hexane/ethyl acetate/dichloromethane (4/1/1) as eluent. Yield: 95 %.

^{1}H NMR ($CDCl_3$, 500MHz, δppm): 7.19-7.29 (m, 10H, Phenyl ring protons), 7.13-7.16 (m, 2H, benzyl ring protons), 6.97-7.02 (m, 2H, benzyl ring proton), 5.53-5.67 (s, 2H, Phe NH), 4.52 (m, 2H, Phe $C^{\alpha}H$), 4.26 (s, 4H, Benzyl CH_2), 2.90-3.10 (m, 4H, Phe $C^{\beta}H$), 1.31 (s, 18H, BOC -CH_3). ^{13}C NMR (125MHz, $CDCl_3$, δ in ppm, 298K): 171.99, 155.62, 137.15, 136.16, 129.56, 128.97, 127.60, 127.37, 126.76 80.03, 56.21, 43.69, 39.41, 29.83, 28.37; ESI-MS (MeOH): m/z (Calc): $C_{34}H_{42}N_4O_6Na$ $[M+Na]^+$653.78; found: 653.86.

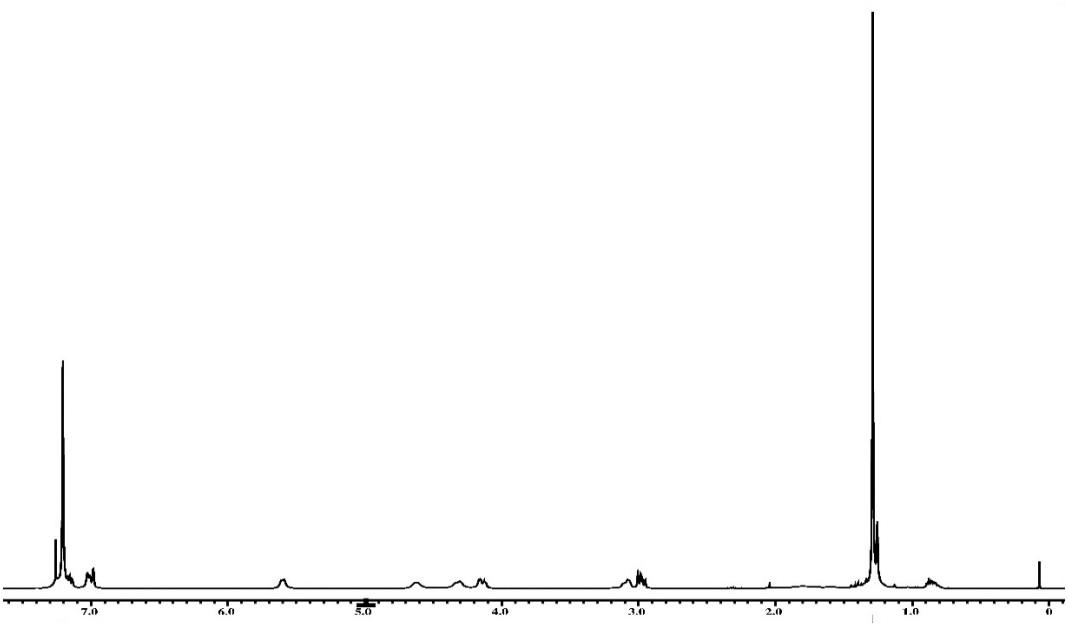

Fig. S10: ^{1}H NMR (500 MHz, $CDCl_3$, δ in ppm, 298K) spectrum of peptide mimetic **2**

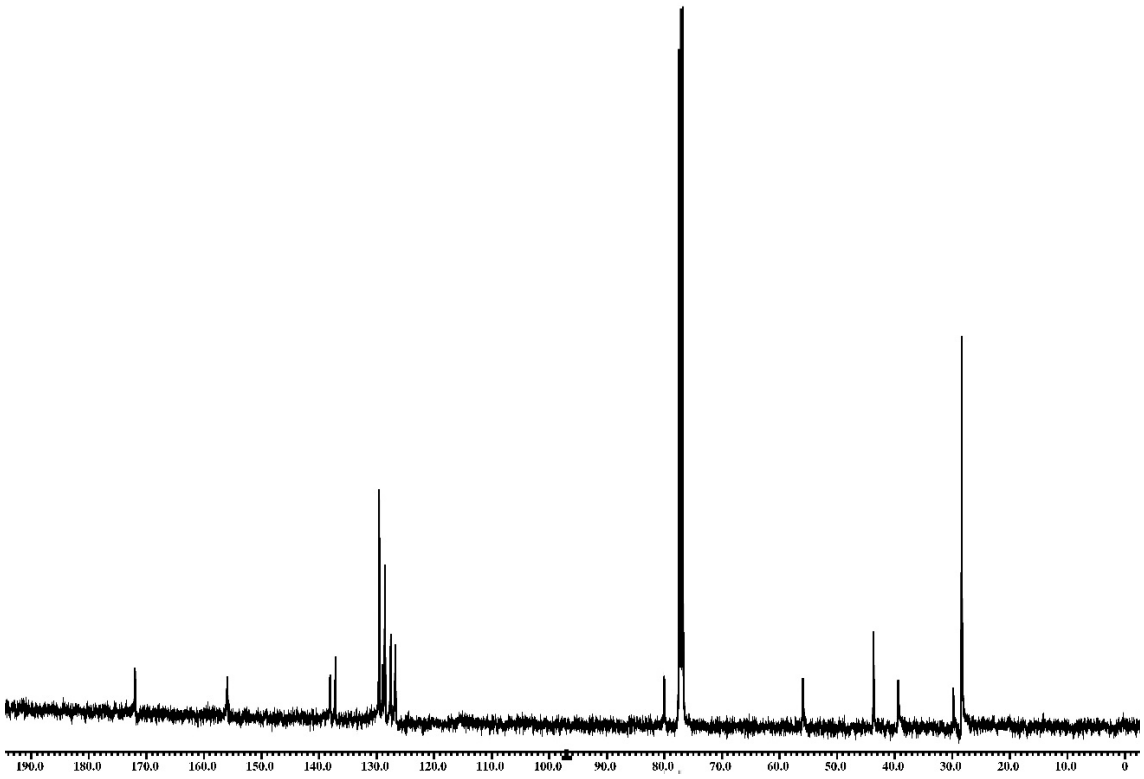

Fig. S11: ^{13}C NMR (125 MHz, $CDCl_3$, δ in ppm, 298K) spectrum of peptide mimetic **2**

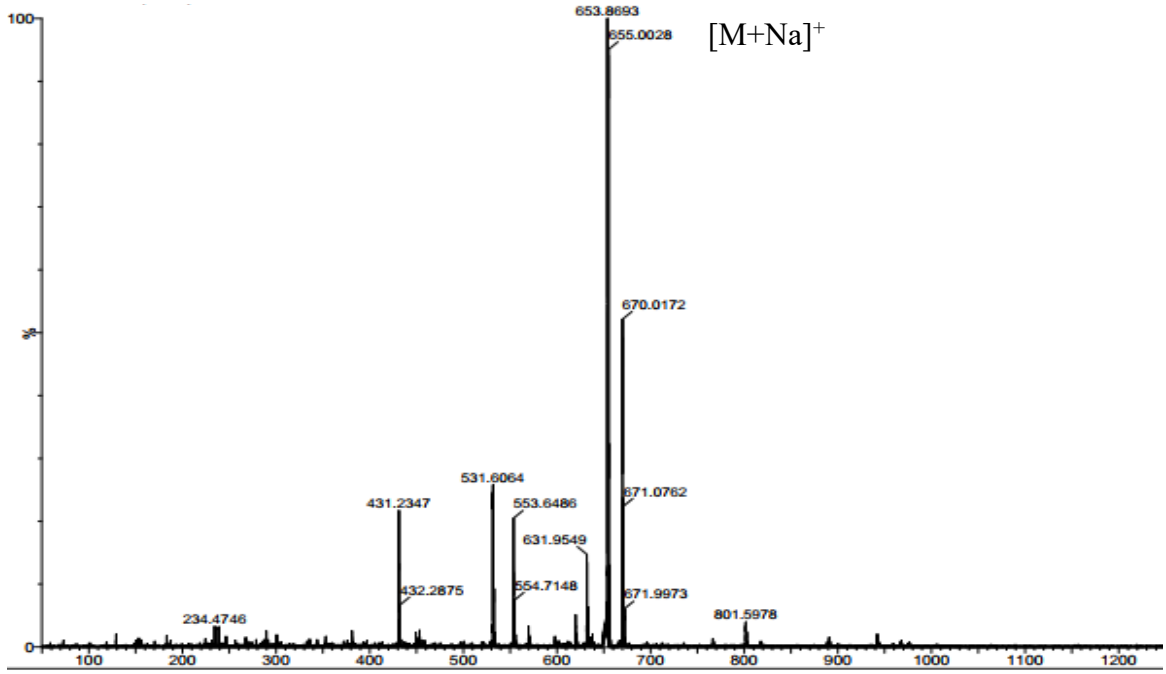

Fig. S12: Mass Spectrum of peptide mimetic **2**

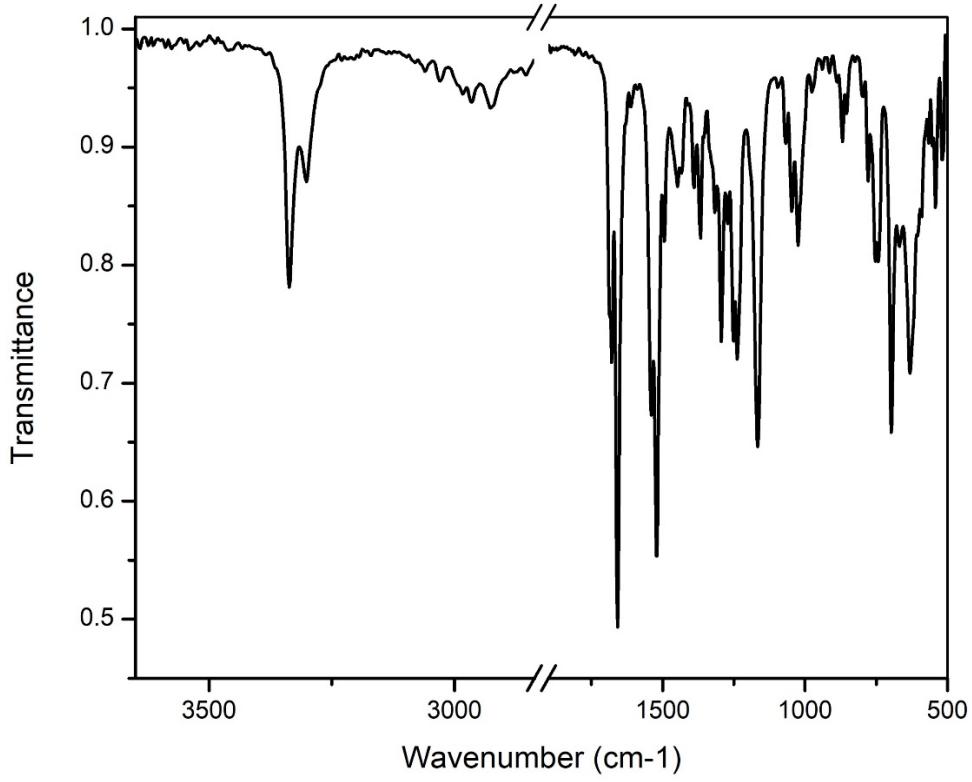

Fig. S13: FT-IR Spectrum of peptide mimetic **2**

Peptide **3**

Boc-phenylalanine 2.653 g (10 mmol) was dissolved in 20 mL of dry DCM and 5 ml of dry DMF under ice−water bath conditions, followed by the addition of 3.095 g (15 mmol) of DCC and 2.297 g (15 mmol) of HOBt. 0.486 g (4.5 mmol) m-phenylenediamine was then added to the solution. The reaction mixture was stirred for 48 h at room temperature. After the completion of the reaction, DCM was evaporated, and the residue was dissolved in ethyl acetate (40 mL) and was put in fridge for 3 h for dicyclohexylurea (DCU) to precipitate, dicyclohexylurea (DCU) was filtered off and water (50 ml) was added and stirred at room temperature for 30 min and subsequently, the ethyl acetate layer was washed with 2 M HCl (3 × 50 mL), brine (2 × 50 mL), 1 M sodium carbonate (3 × 50 mL), and brine (2 × 50 mL), respectively. The organic layer was dried over anhydrous sodium sulfate and evaporated under vacuum to yield peptide **3** as powdery form. The product was purified by silica gel using hexane/ethyl acetate (4/1) as eluent. Yield: 90 %.

^{1}H NMR ($CDCl_3$, 500MHz, δppm): 8.63 (s, 2H, Benzyl NH), 7.51 (s, 1H, Benzyl proton) 7.20-7.35 (m, 10H, Phenyl ring protons), 7.04-7.19 (m, 3H, benzyl ring protons), 5.51 (s, 2H, Phe NH), 4.67 (m, 2H, Phe $C^{\alpha}H$), 2.90-3.15 (m, 4H, Phe $C^{\beta}H$), 1.42 (s, 18H, BOC -CH_3). ^{13}C NMR (125MHz, $CDCl_3$, δ in ppm, 298K): 171.02, 156.02, 138.04, 136.14, 129.50, 128.87, 127.24, 112.41, 110.89, 80.08, 54.23, 38.21, 28.83; ESI-MS (MeOH): m/z (Calc): $C_{36}H_{46}N_4O_6Na$ $[M+Na]^+$ 626.30; found: 626.65.

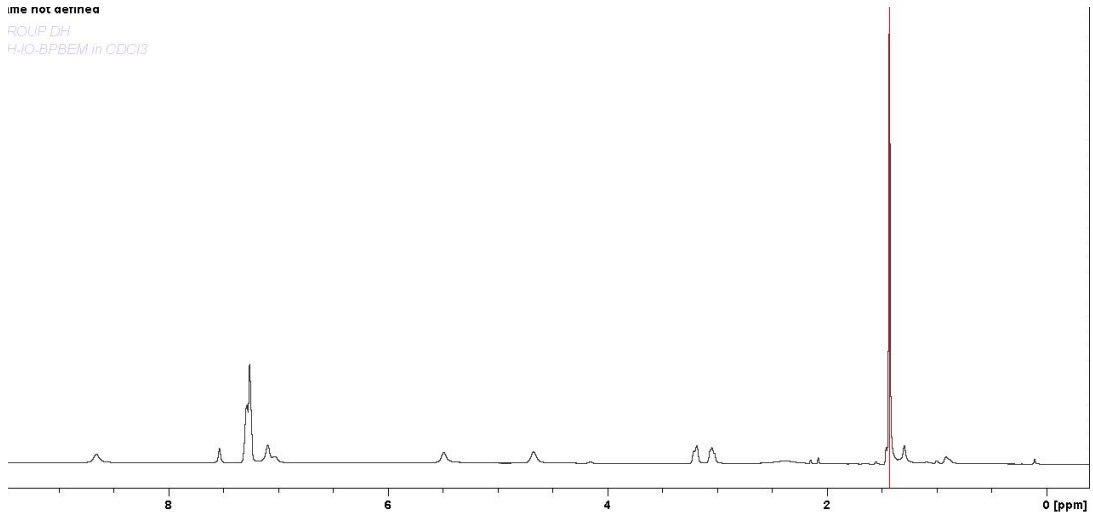

Fig. S14: ^{1}H NMR (500 MHz, $CDCl_3$, δ in ppm, 298K) spectrum of peptide mimetic **3**

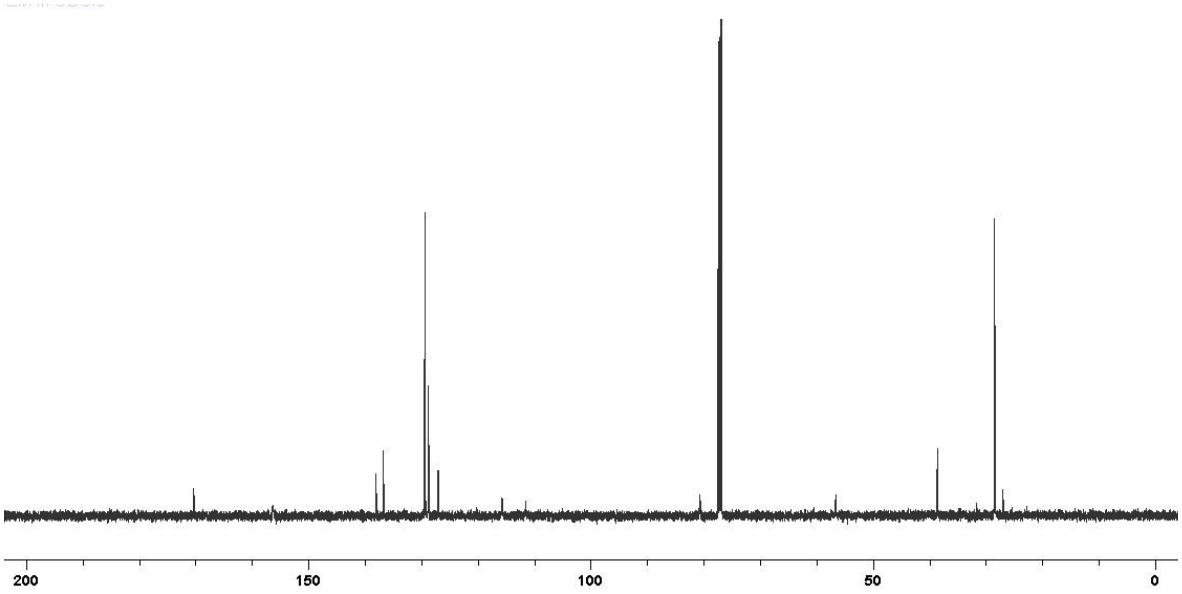

Fig. S15: ^{13}C NMR (125 MHz, $CDCl_3$, δ in ppm, 298K) spectrum of peptide mimetic **3**

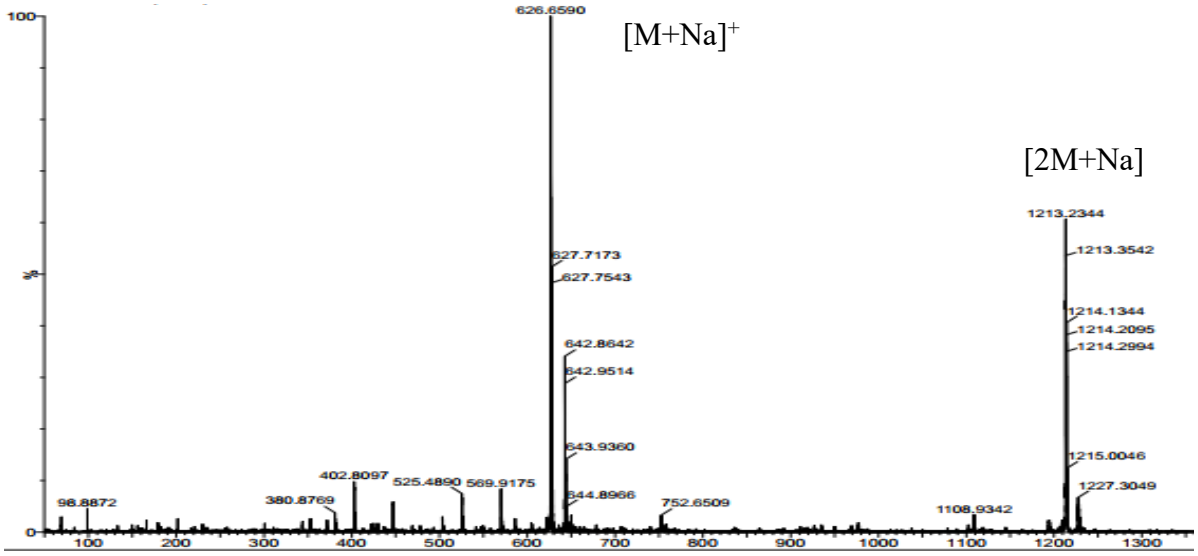

Fig. S16: Mass Spectrum of peptide mimetic **3**

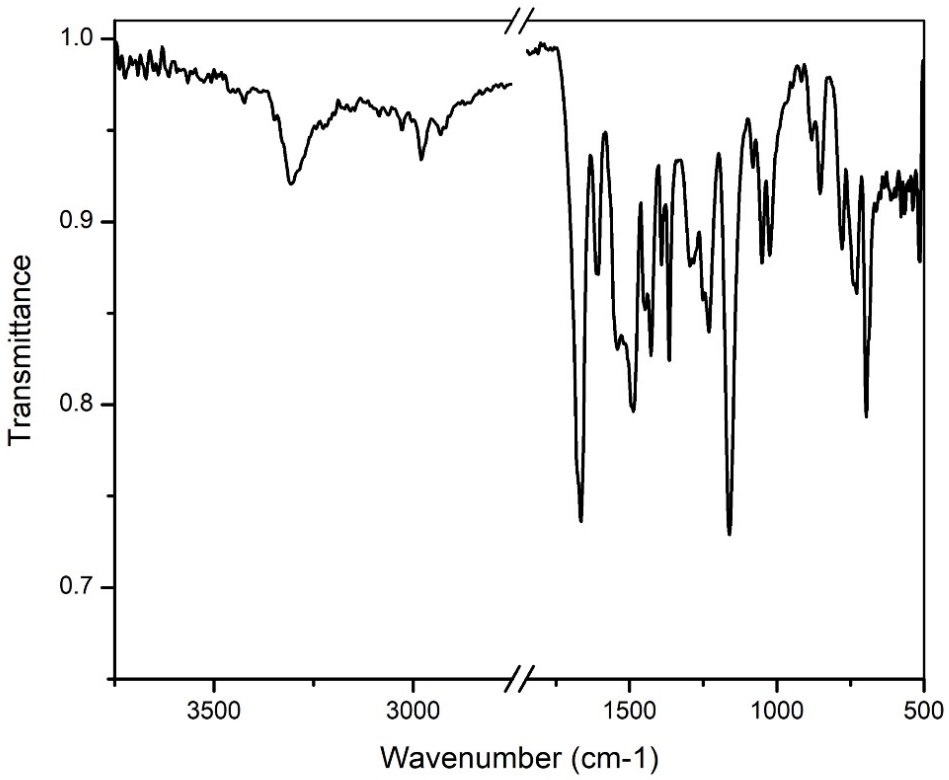

Fig. S17: FT-IR Spectrum of peptide mimetic **3**