

## Electronic Supplementary Information

### **Self assembly and Hydrogelation of Spermine Functionalized Aromatic Peptidomimetics Against Planktonic and Sessile Methicillin Resistant *S. aureus***

\*Correspondence should be addressed to:

Dr. Santosh Pasha,

Peptide Research Laboratory,

CSIR-Institute of Genomics and Integrative Biology,

Mall Road, Delhi, India

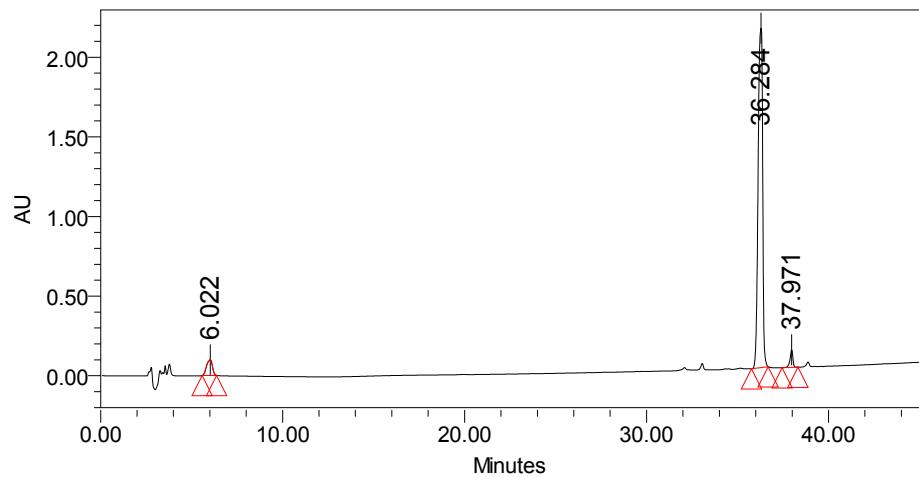
E-mail: [spasha@igib.res.in](mailto:spasha@igib.res.in)

Tel: 91-011-27666156 (170);

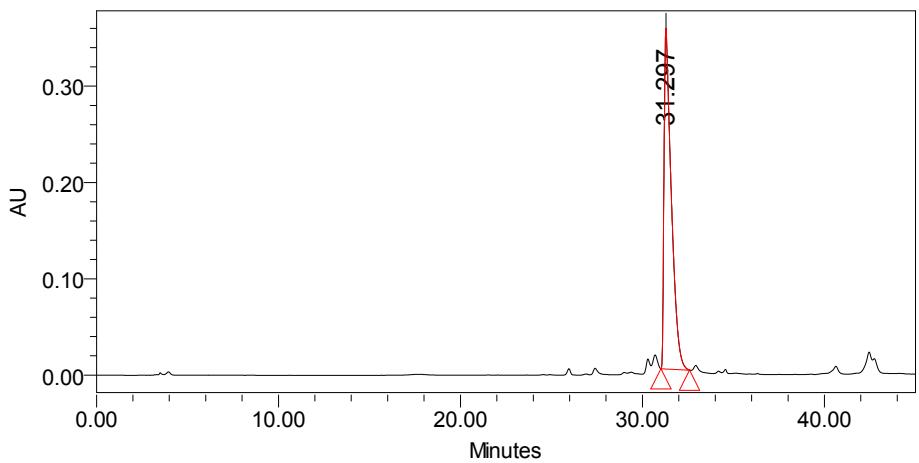
Fax: +91 11 27667471

#### **HPLC chromatograms of all peptides**

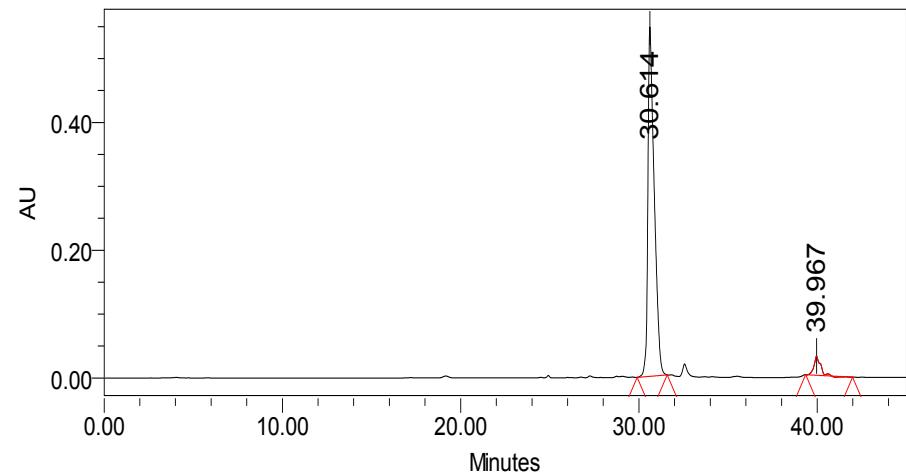
For peptides RP-HPLC chromatograms (absorbance at 220 nm) are reported. A linear gradient of 10 to 90% buffer 2 was run from 5 to 40 min. and gradient was reversed 90 to 10% of buffer 2 between 40-45 min for equilibration. Here buffer 1 was water (0.1 % TFA) and buffer 2 was acetonitrile (0.1% TFA) over 45 minutes.



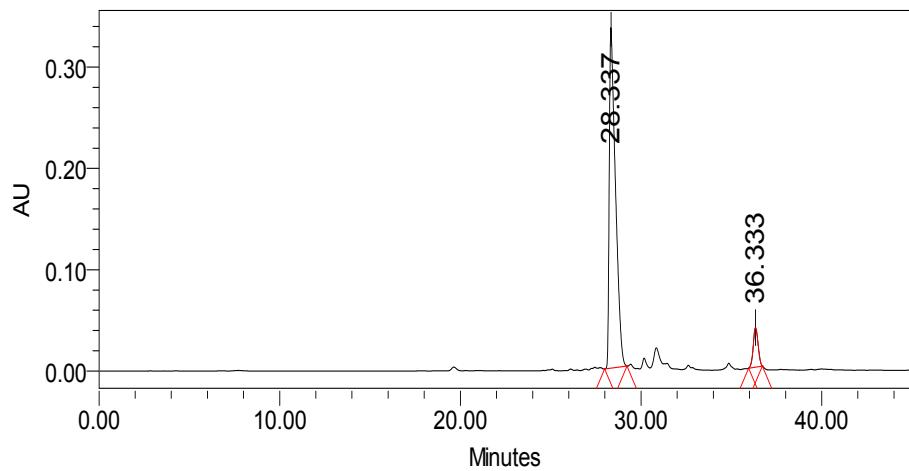
**Fig S1** HPLC chromatogram of NF-1



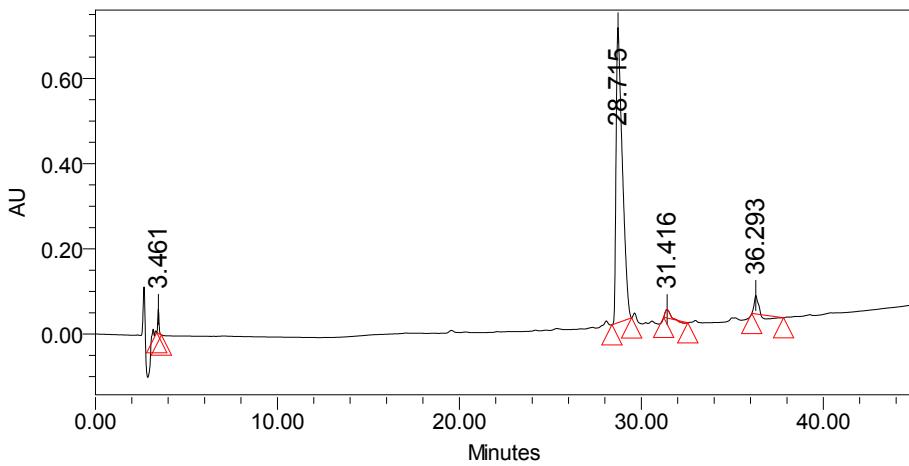
**Fig S2** HPLC chromatogram of NF-2



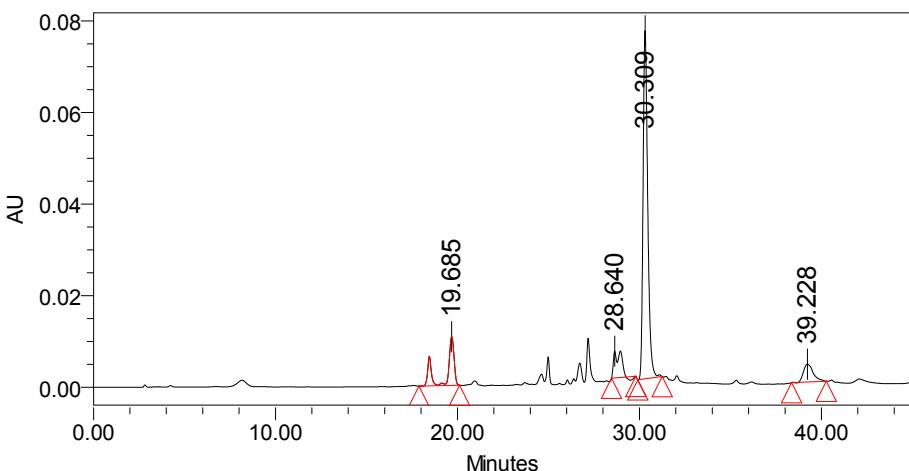
**Fig S3** HPLC chromatogram of NF-3



**Fig S4** HPLC chromatogram of NF-4



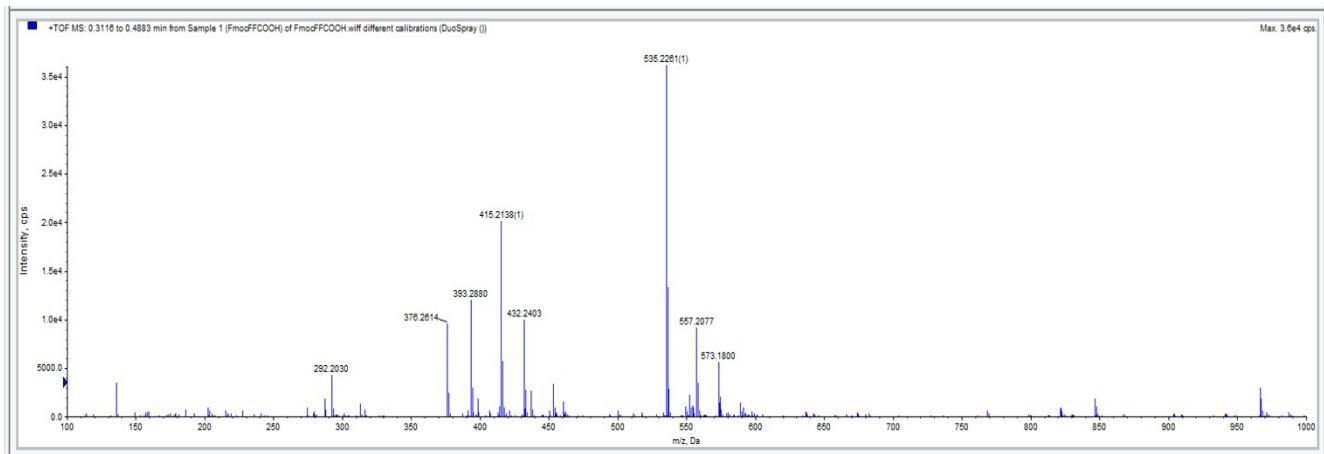
**Fig S5** HPLC chromatogram of NF-5



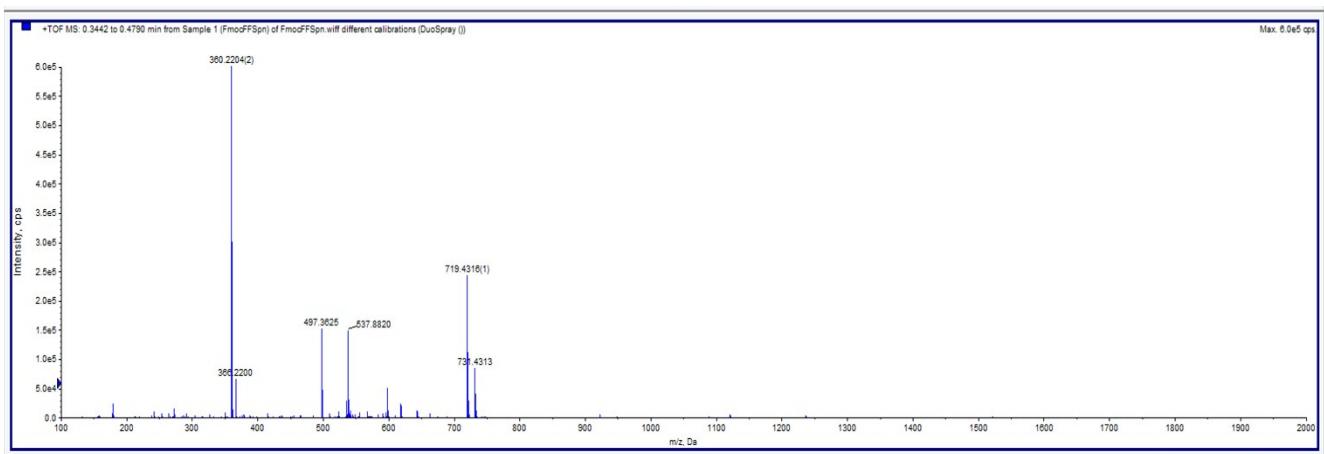
**Fig S6** HPLC chromatogram of NF-6

## ESI-MS spectra of peptides

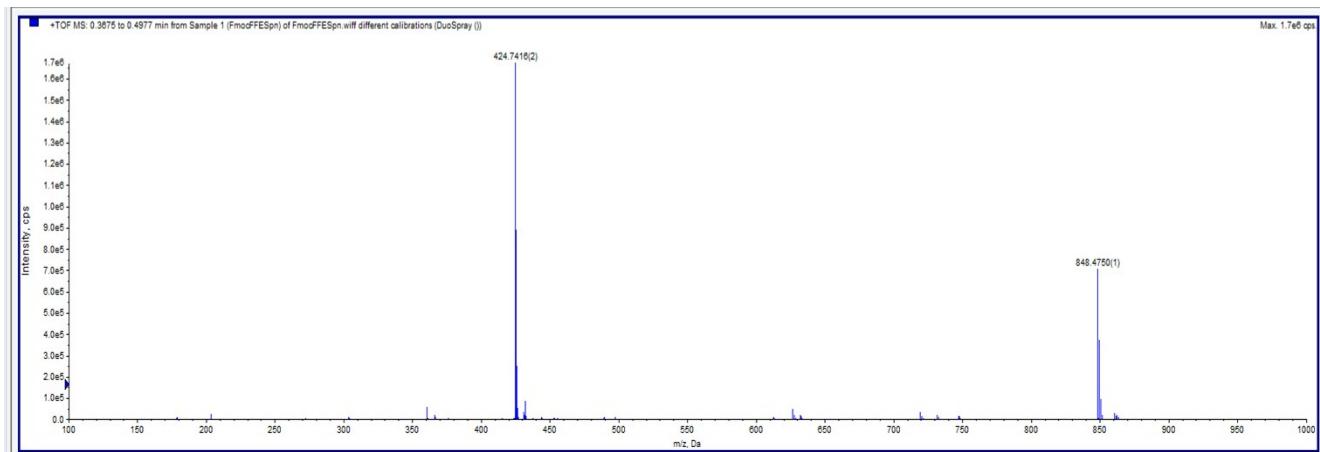
All spectra were acquired by direct infusion of liquid samples (in methanol) in ESI-MS, TripleTOF® 5600, AB Sciex. The MS was run in positive ion mode with capillary voltage: 5.5 kV and curtain gas: 25 Ltr/h.



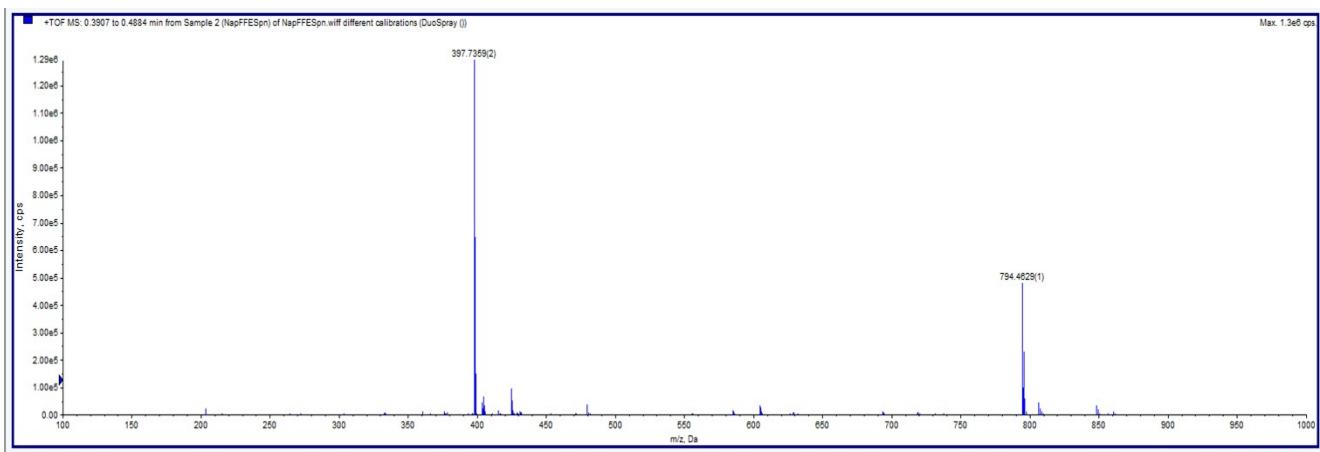
**Fig S7** ESI-MS of NF-1



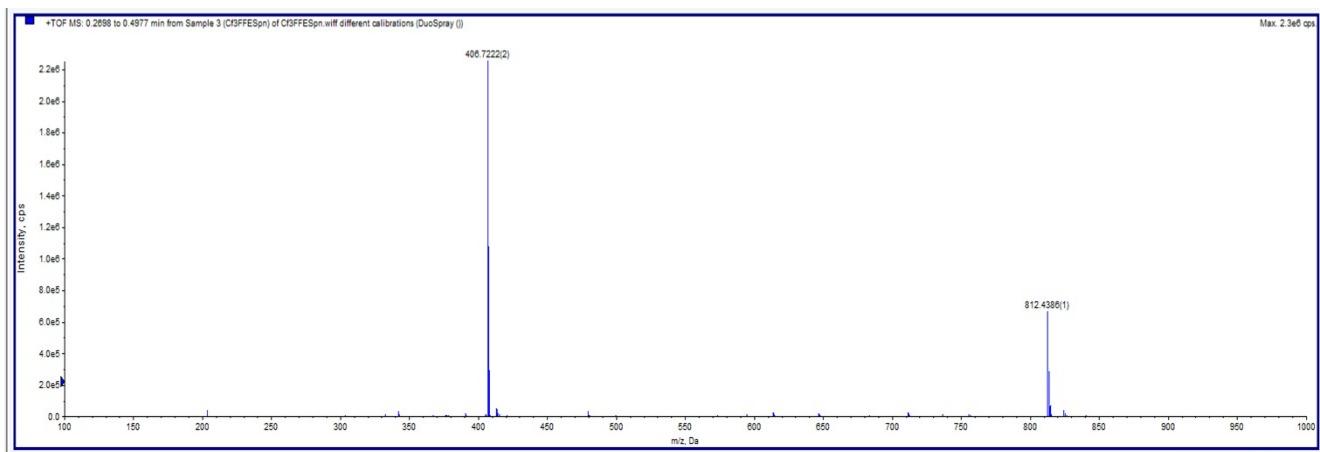
**Fig S8** ESI-MS of NF-2



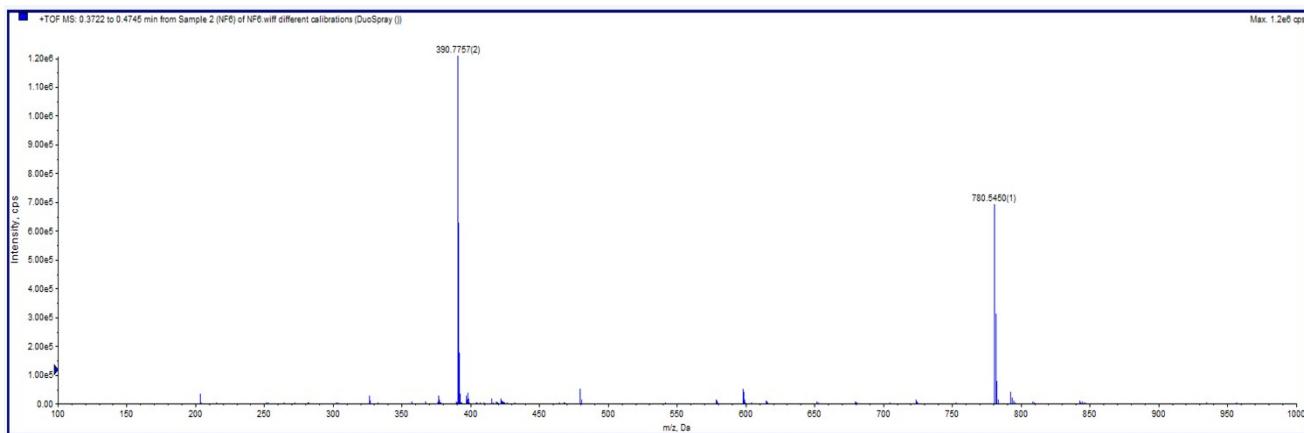
**Fig S9** ESI-MS of NF-3



**Fig S10** ESI-MS of NF-4



**Fig S11** ESI-MS of NF-5

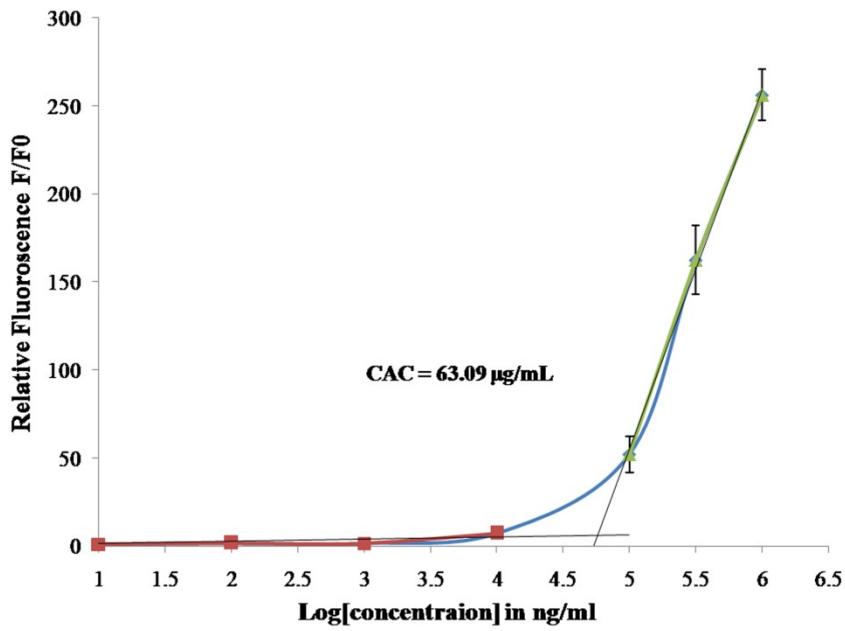


**Fig S12** ESI-MS of NF-6

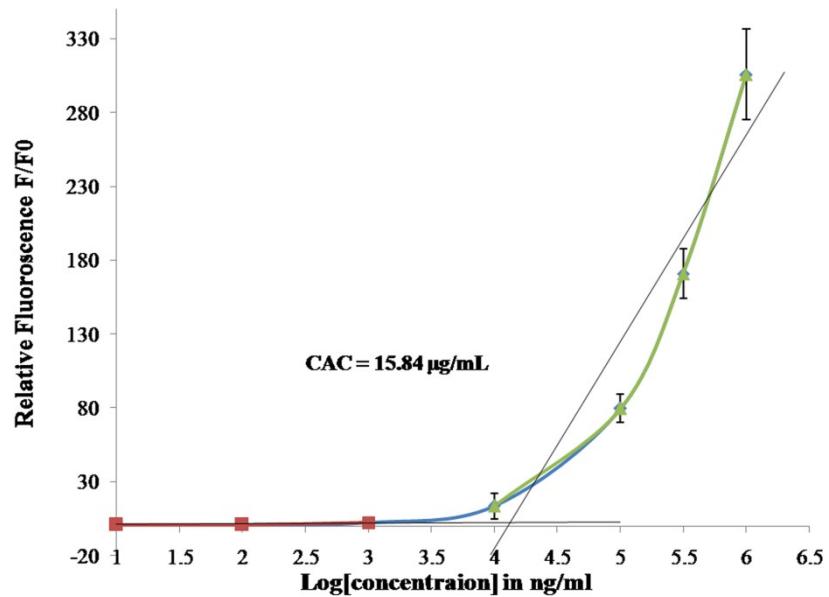
### Critical Aggregation Concentrations of Peptides in MHB media

**Method:** CAC values of designed peptidomimetics were determined using static light scattering (SLS) measurements on a spectrofluorometer (Jobin Yvon, FluoroMax-4; Horiba Scientific, Edison, NJ, USA) as described previously.<sup>1</sup> Briefly, the lyophilized peptidomimetics were dispersed at 2% w/v in MQ water at room temperature. The sample was diluted 2 fold in Mueller-Hinton broth Media (growth medium as used for MIC determination). Further, serial ten-fold dilutions of the peptidomimetics were prepared in the same medium to get concentrations in the range of (1000-0.001  $\mu$ g/mL). The samples were subjected to light scattering using 90° geometry to collect the scattering intensity at 402 nm upon excitation of sample at 410 nm. Slit widths for both excitation and emission were fixed at 2.5 nm. For determination of CAC, intensities of scattered signal were plotted against peptidomimetics concentration. CAC was determined from the inflection point which was defined as the abscissa where the intensity rises steeply.

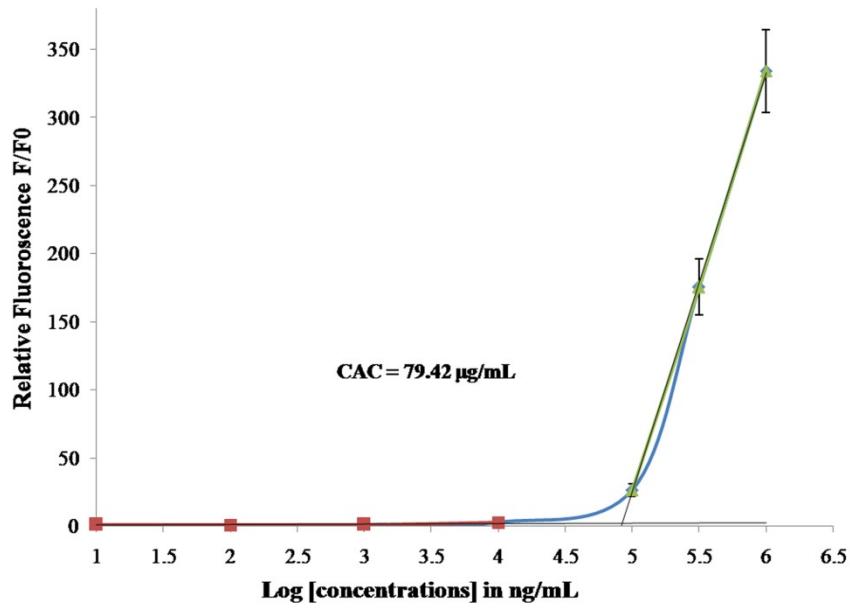
Following figures describes Critical aggregation concentration determination of peptides by static light scattering intensity. Relative fluorescence was plotted against log concentration of peptides. Here,  $F$  represents fluorescence intensity at a fixed peptide concentrations and  $F_0$  is fluorescence Intensity of MHB only.



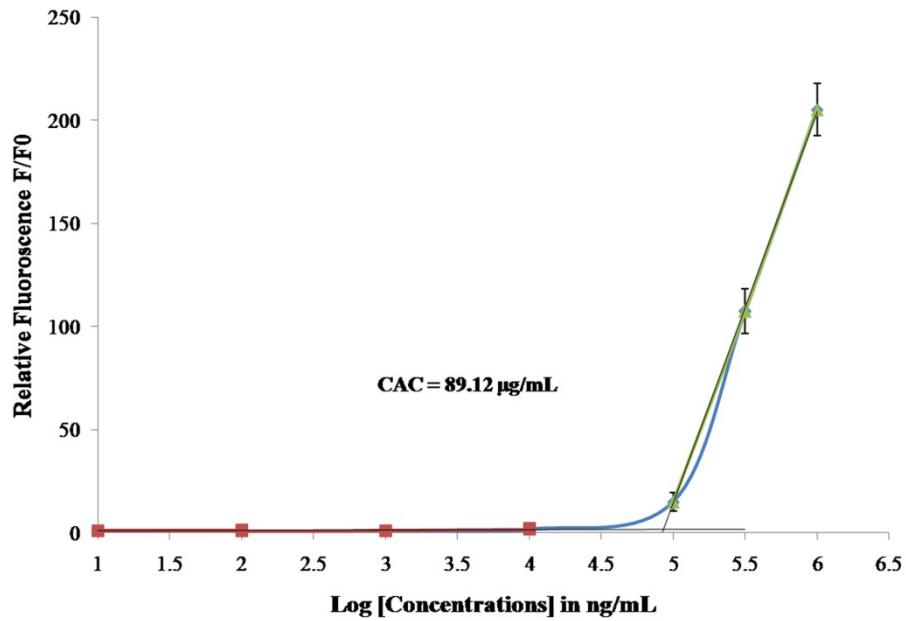
**Fig S13:** CAC determination graph of NF-2



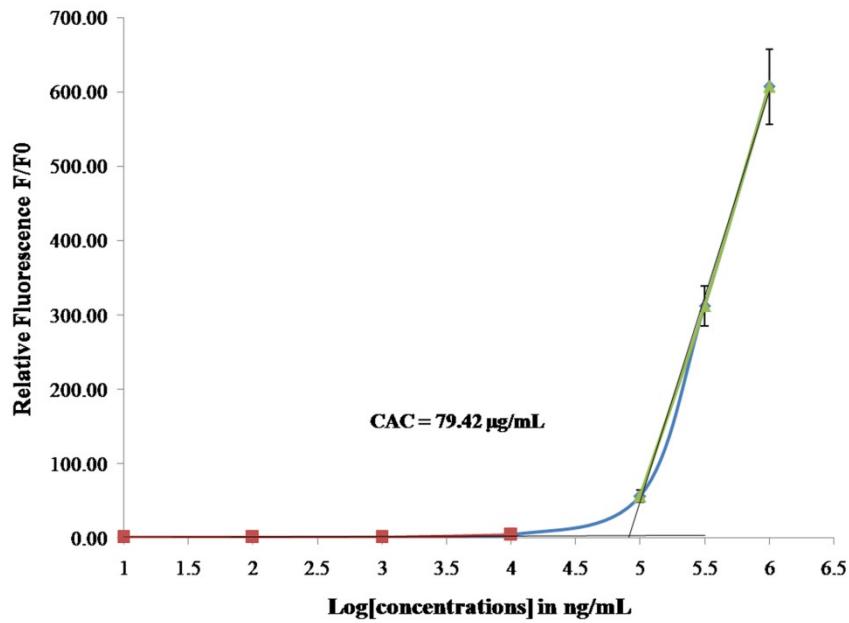
**Fig S14:** CAC determination graph NF-3



**Fig S15:** CAC determination graph NF-4



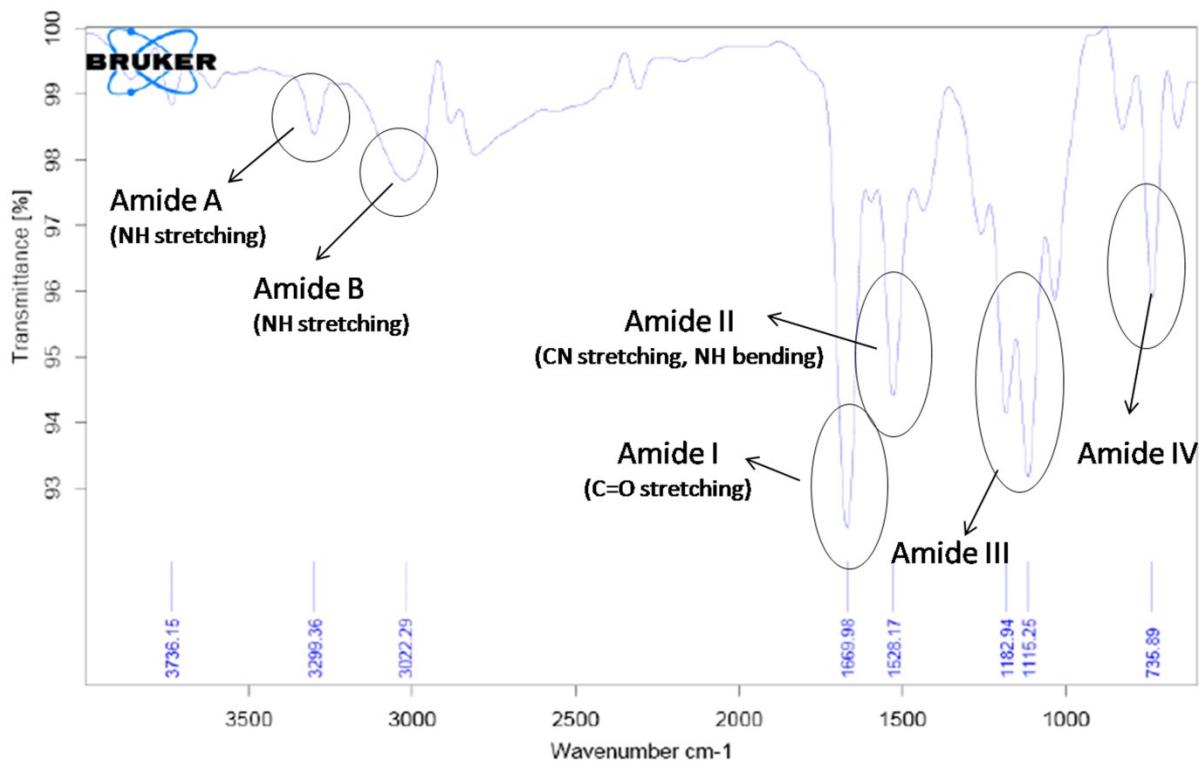
**Fig S16:** CAC determination graph NF-5



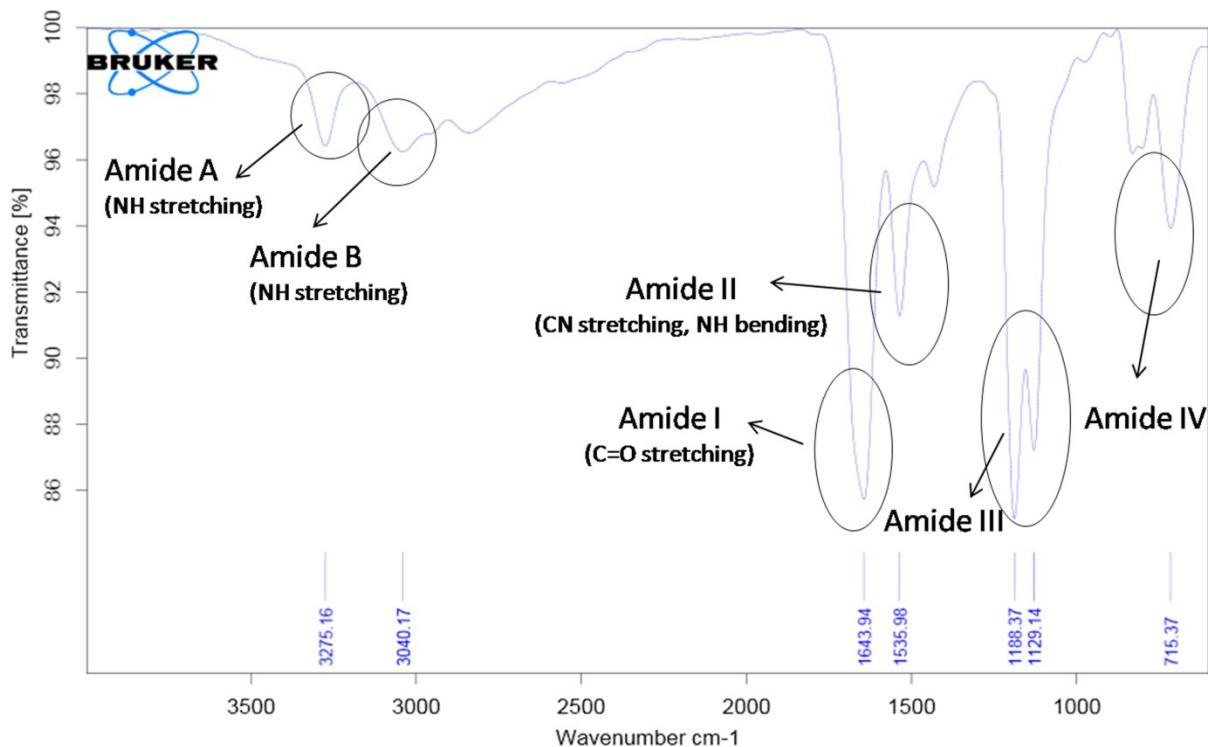
**Fig S17:** CAC determination graph NF-6

### FTIR spectrum of peptides

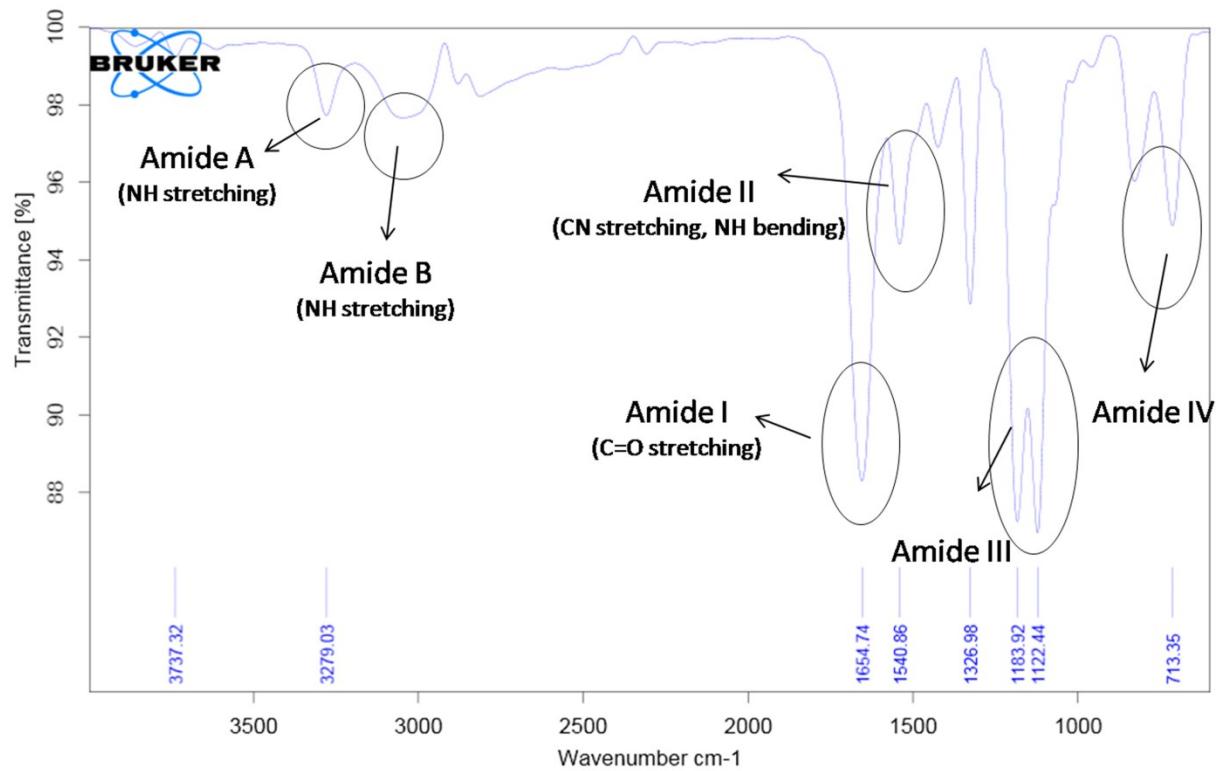
FTIR spectrum of peptides of xerogel (lyophilized dried gel).



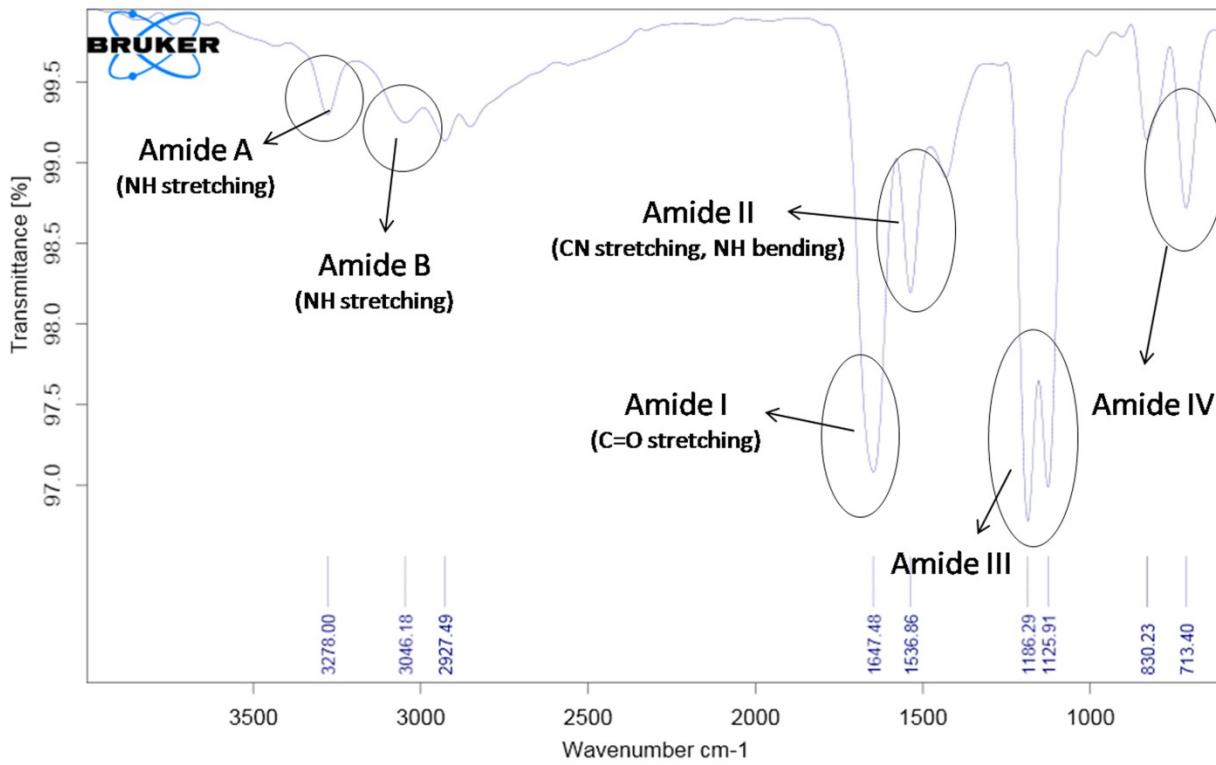
**Fig S18:** FTIR spectrum of NF-3



**Fig S19:** FTIR spectrum of NF-4



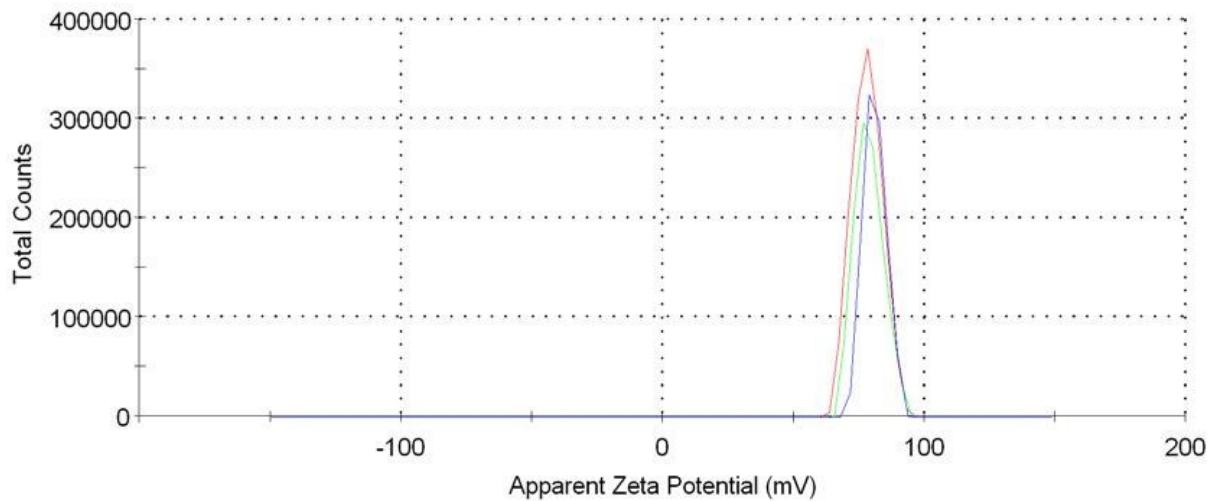
**Fig S20:** FTIR spectrum of NF-5



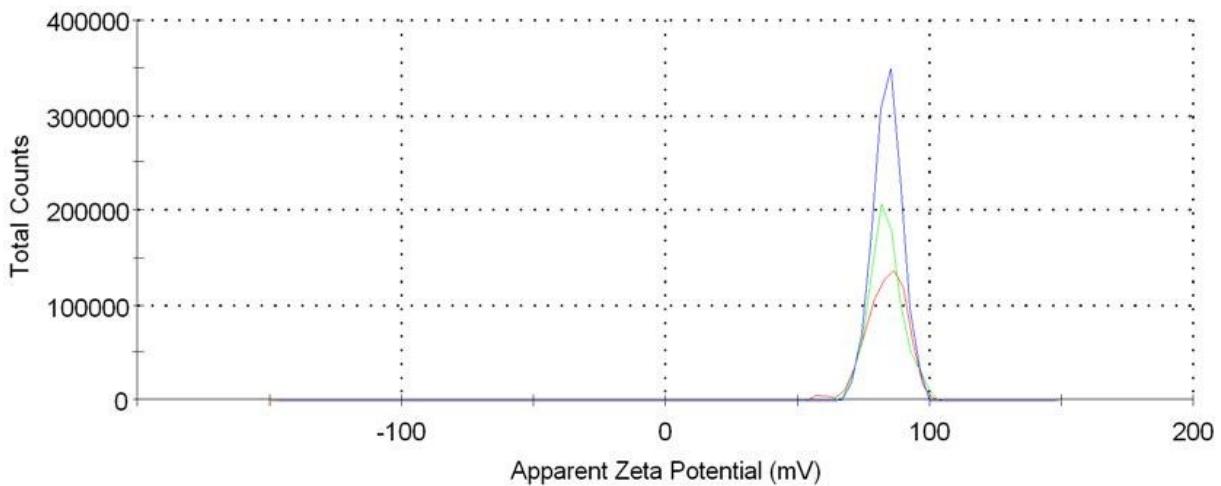
**Fig S21:** FTIR spectrum of NF-6

### Surface zeta potential measurement of hydrogel nanofibres

Surface zeta potential was obtained by using zetasizer at concentrations of NF-3 and NF-4 at 0.1% w/v concentrations in water.



**Fig S22:** Surface zeta potential of NF-3



**Fig S23:** Surface zeta potential of NF-4

### REFERENCES:

1. M. M. Konai, C. Ghosh, V. Yarlagadda, S. Samaddar and J. Haldar, *Journal of Medicinal Chemistry*, 2014, **57**, 9409-9423.