Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Biomimetic Design: A Programmed Tetradecapeptide Folds and Homodimerizes as a Stereochemically Articulated Receptor Protein

Punam Ghosh, Deepa Pedenekar, and Susheel Durani[a*]

[a]Department of Chemistry, Indian Institute of Technology Bombay, Mumbai-400076, India

*CORRESPONDING AUTHOR EMAIL: sdurani@iitb.ac.in

*CORRESPONDING AUTHOR FOOTNOTE

Dr. S. Durani (Professor),

Department of Chemistry,

Indian Institute of Technology Bombay,

Mumbai-400076, India

Email: sdurani@iitb.ac.in

Ph: +91-22-25767164

Fax: +91-22-25767152

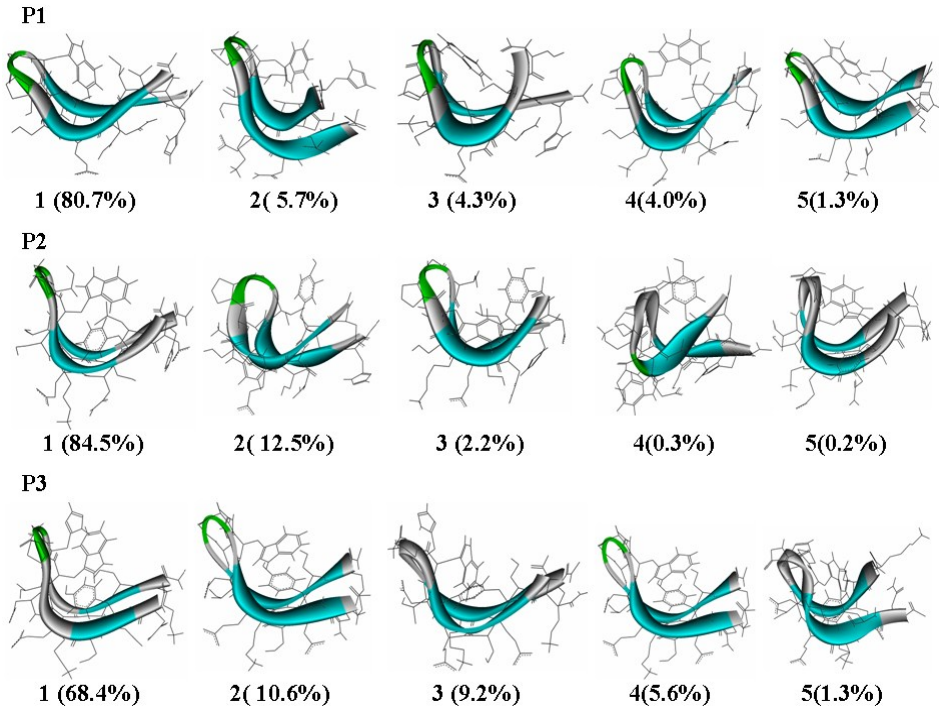


Figure S1: Ribbon representation of central member of the five most populous clusters of monomer fold in 50 ns-MD trajectory enumerated to 0.15 nm RMSD cut-off over Cα atoms of polypeptide. % Population of the ensemble in each cluster is shown in parenthesis.

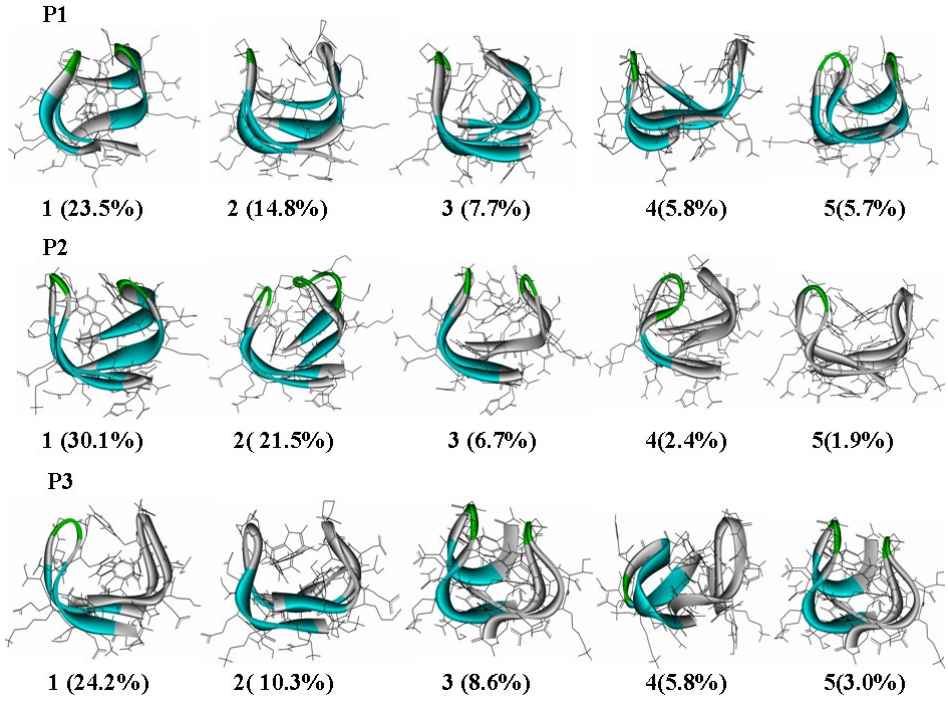


Figure S2: Ribbon representation of central member of the five most populous clusters of homodimer fold in 50 ns-MD trajectory enumerated to 0.15 nm RMSD cut-off over Cα atoms of polypeptides. % Population of the ensemble in each cluster is shown in parenthesis.

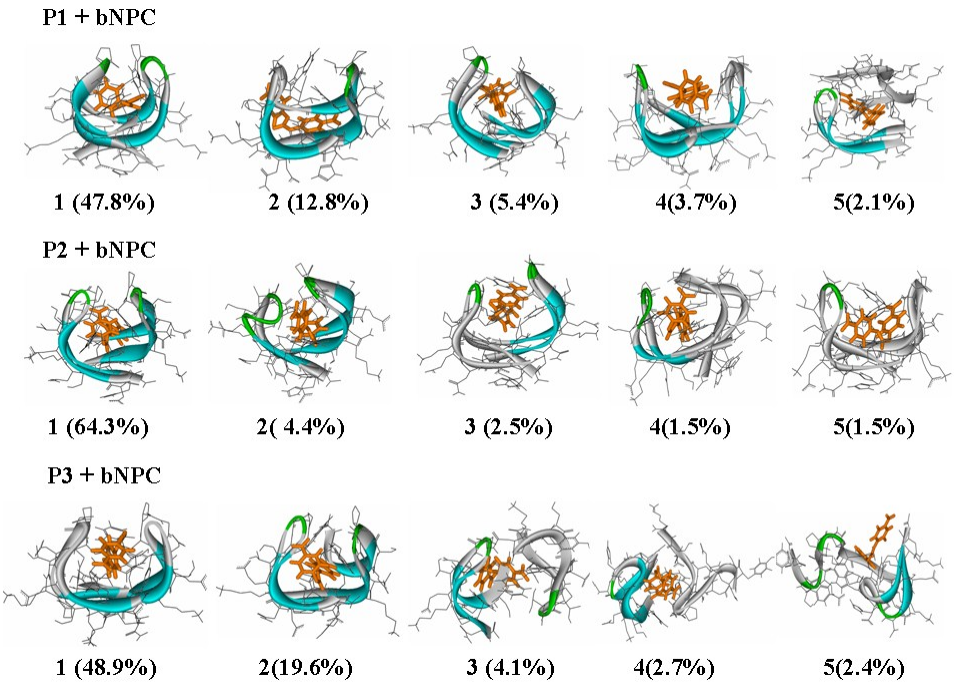


Figure S3: Ribbon representation of central member of the five most populous clusters of the bNPC-bound homodimer in 50 ns-MD trajectory enumerated to 0.15 nm RMSD cut-off over Cα atoms of the polypeptide. % Population of the ensemble in each cluster is shown in parenthesis.

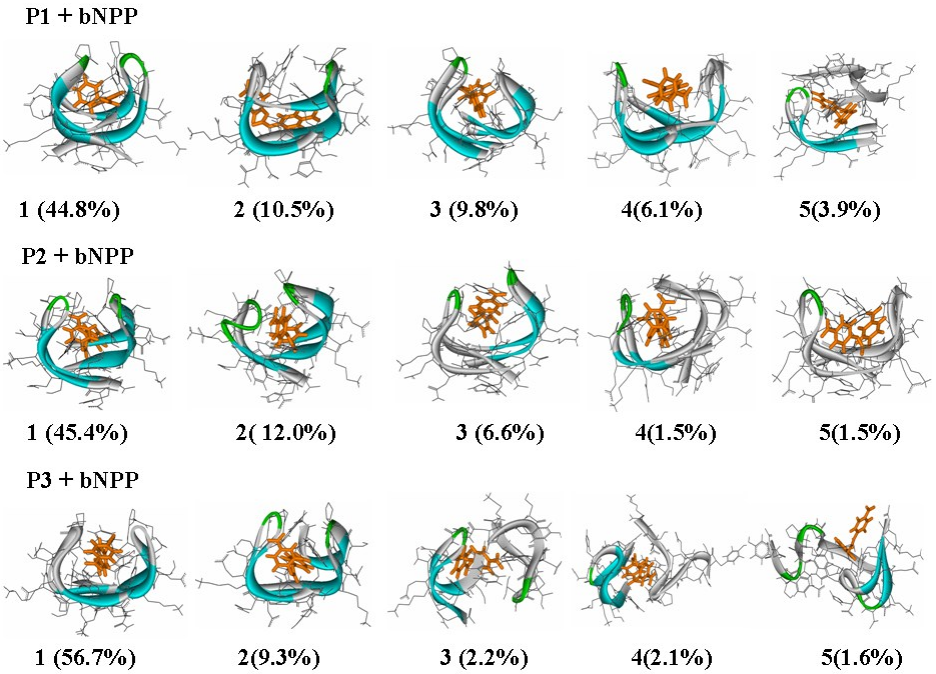
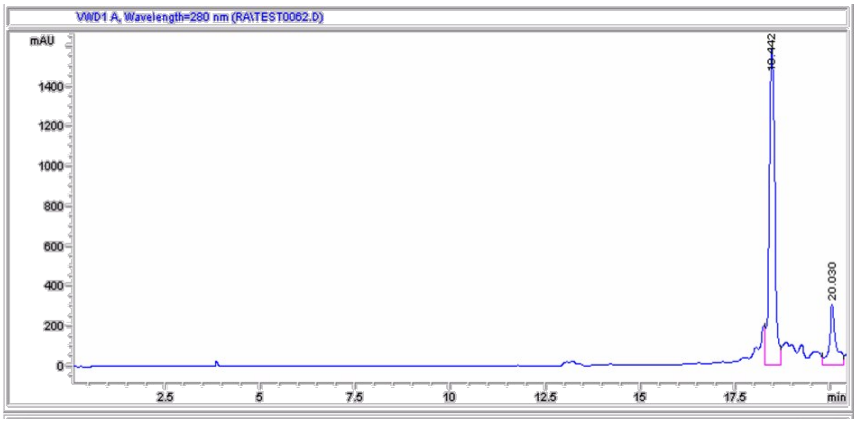
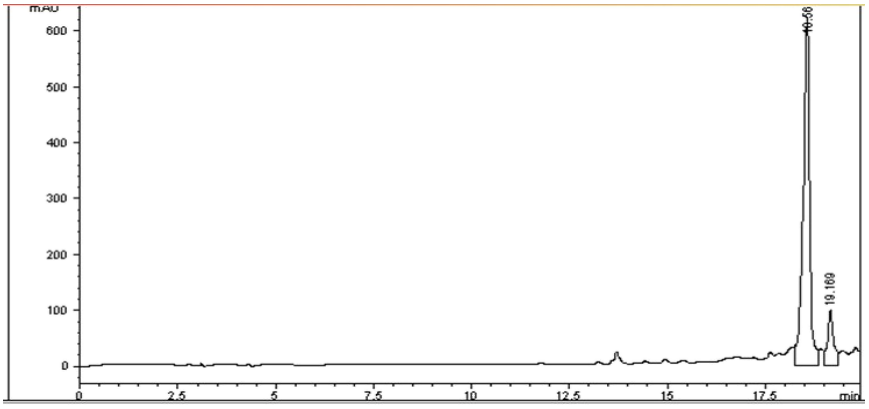


Figure S4: Ribbon representation of central member of the five most populous clusters of the bNPP-bound homodimer in 50 ns-MD trajectory enumerated to 0.15 nm RMSD cut-off over Cα atoms of polypeptides. % Population of the ensemble in each cluster is shown in parenthesis.

P1



P2



P3

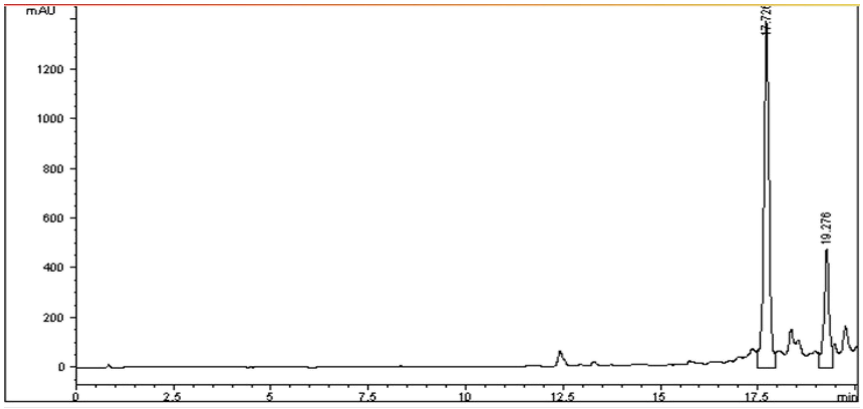
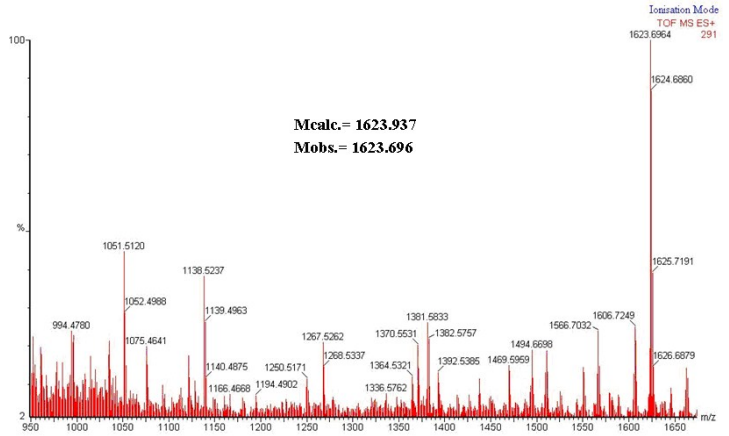


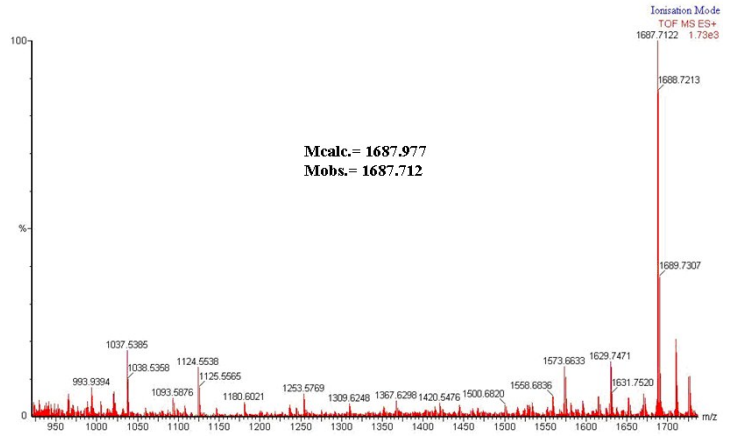
Figure S5: HPLC profiles showing the purity of the peptides P1, P2 and P3

P1



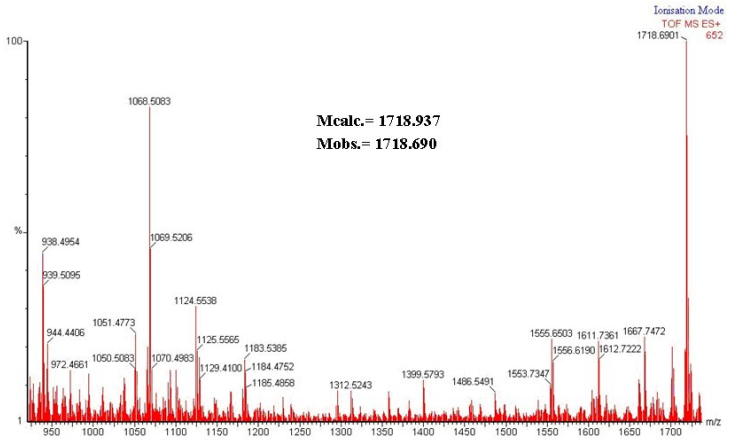
Panel A

P2



Panel B

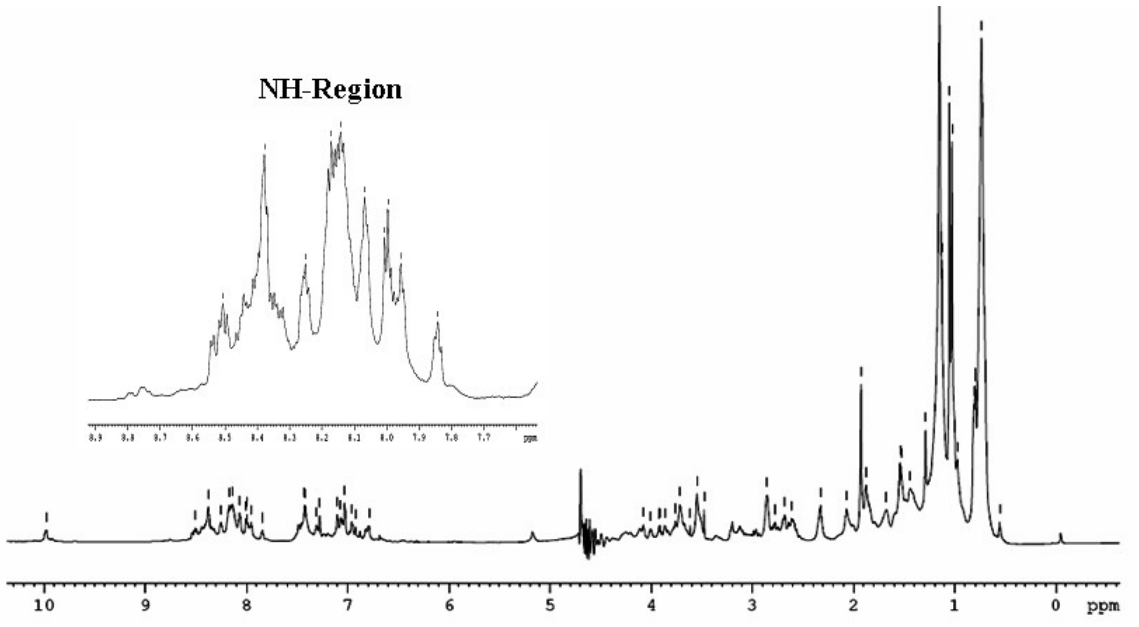
P3



Panel C

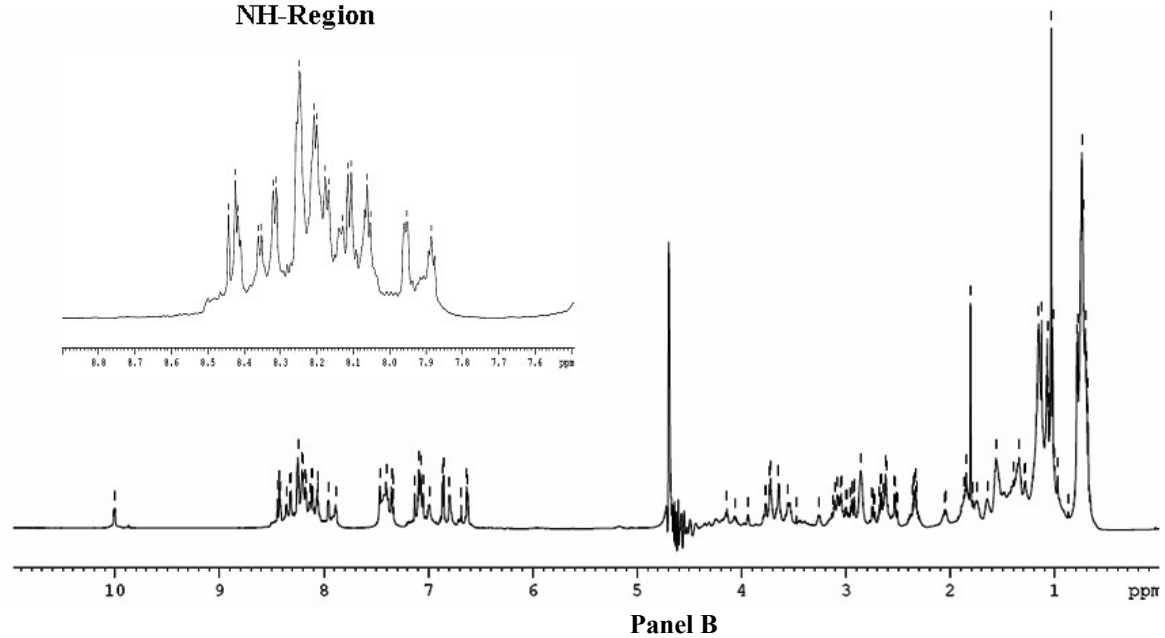
Figure S6: ESI Mass Spectra of the peptides

P1



Panel A

P2



Panel B

P3

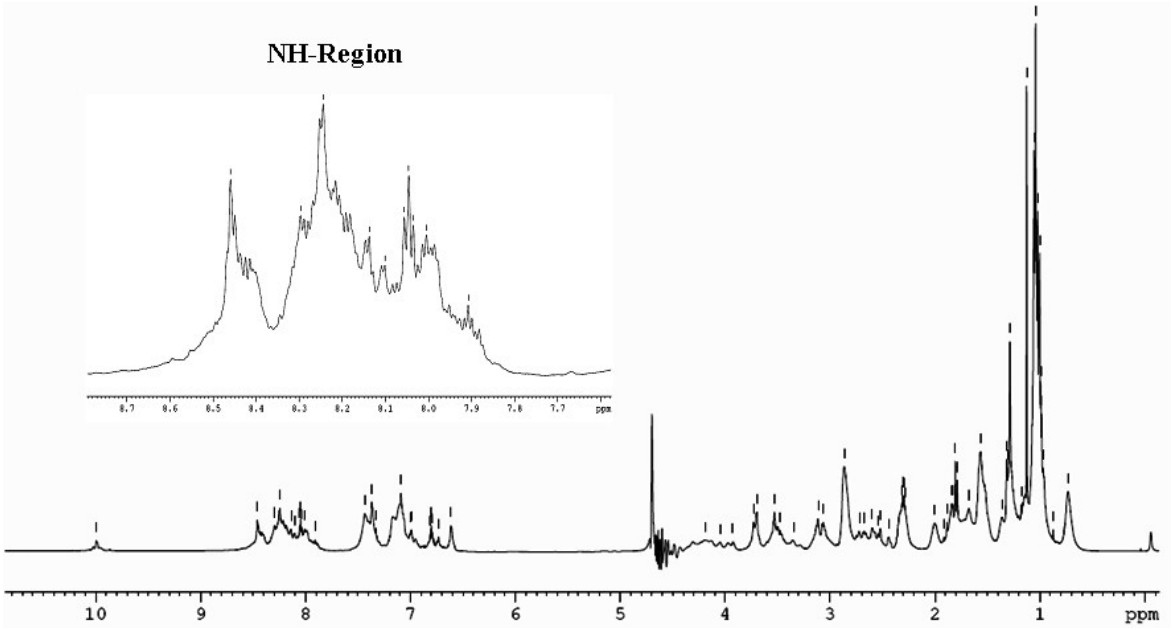


Figure S7: ^{1}H-NMR spectra of **P1** (Panel A) **P2** (Panel B) and **P3** (Panel C) recorded at 800 Mz in 90% D_2O-H_2O mixture. Expanded NH regions are shown as insets.

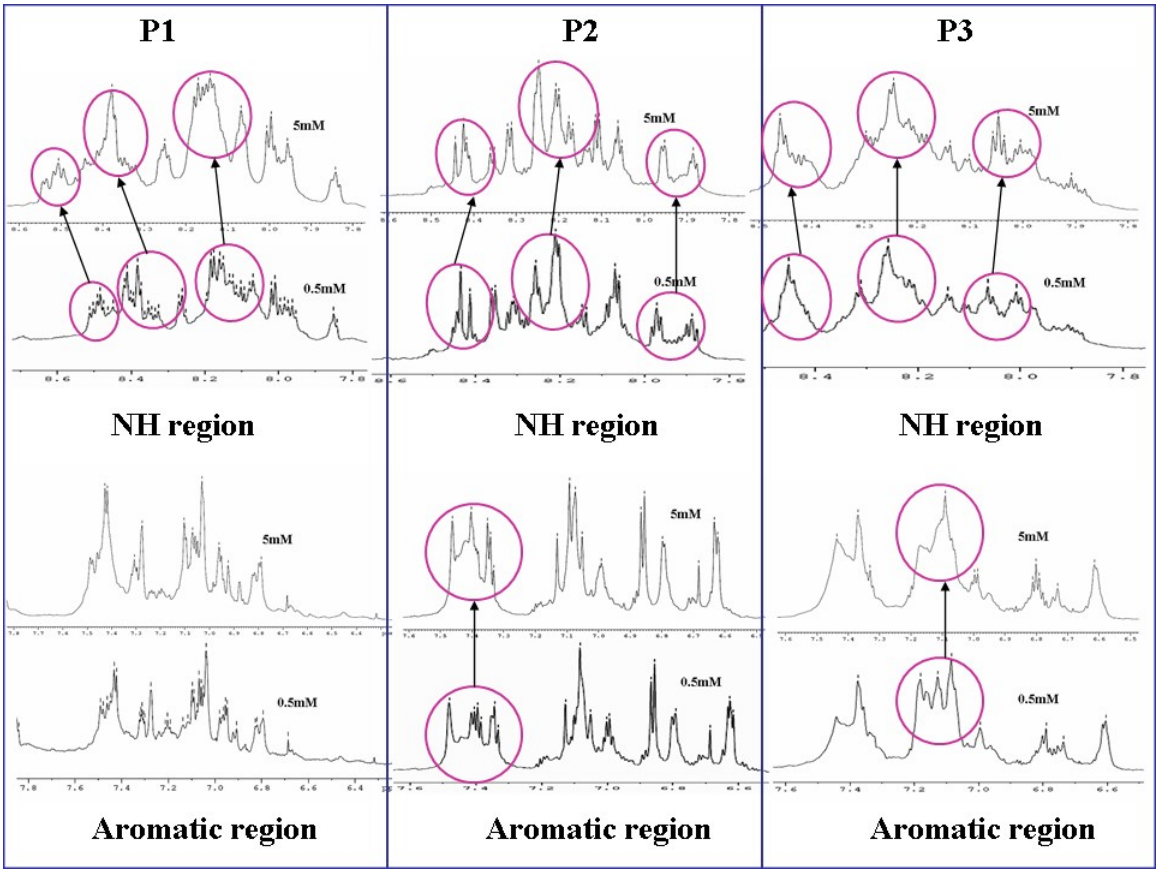


Figure S8: Peptide-NH and Aromatic-H regions of ^{1}H-NMR spectra recorded at 0.5 mM and 5.0 mM concentrations of the peptides in 90% D_2O-H_2O mixture. The specific resonances affected by dilution are highlighted with circles.

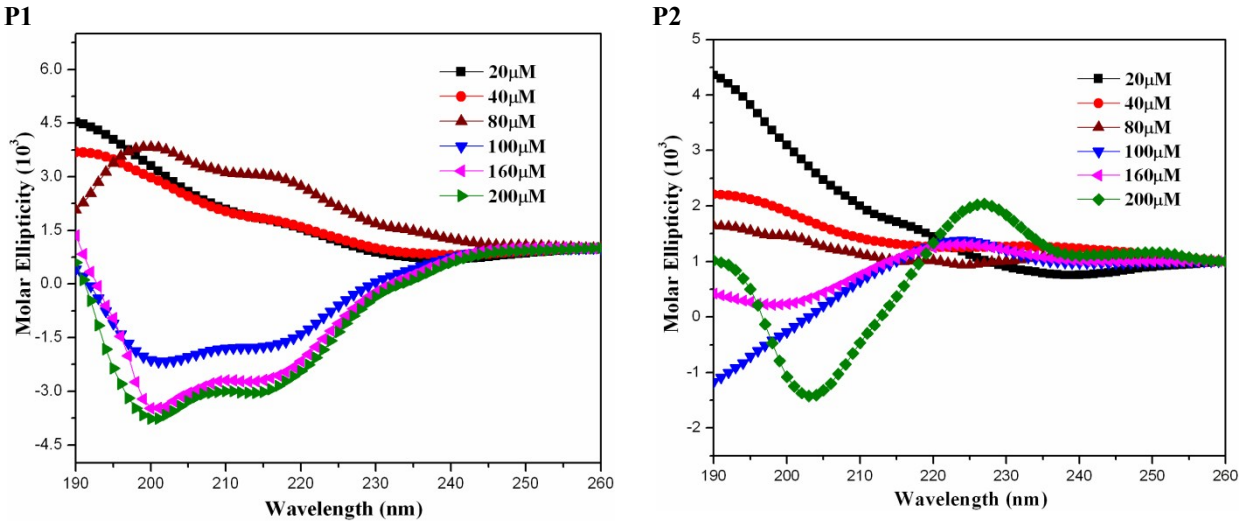


Figure S9: CD traces of **P1** (Left Panel) and **P2** (Right Panel) recorded in water in the concentration range 20-200 μM.

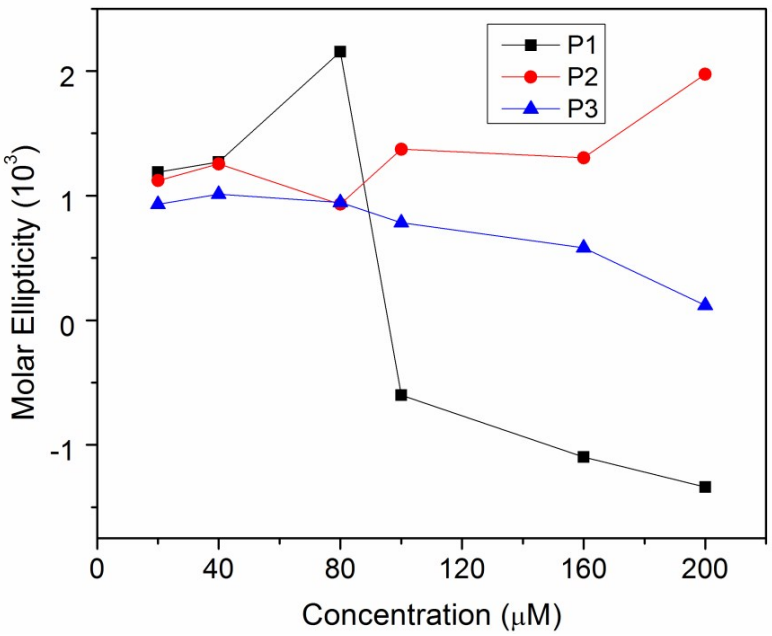
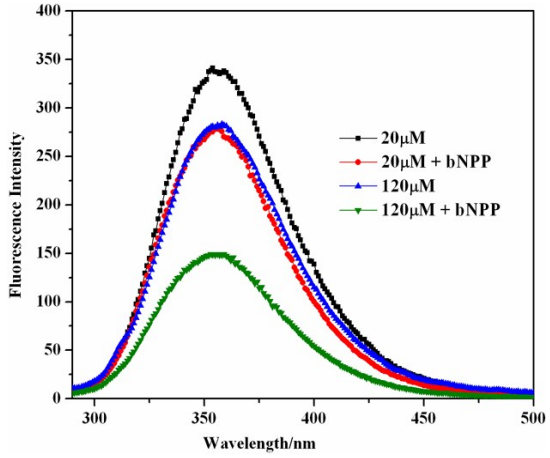


Figure S10: Molar ellipticty vs concentration plots for peptides **P1**, **P2** and **P3** recorded in water.



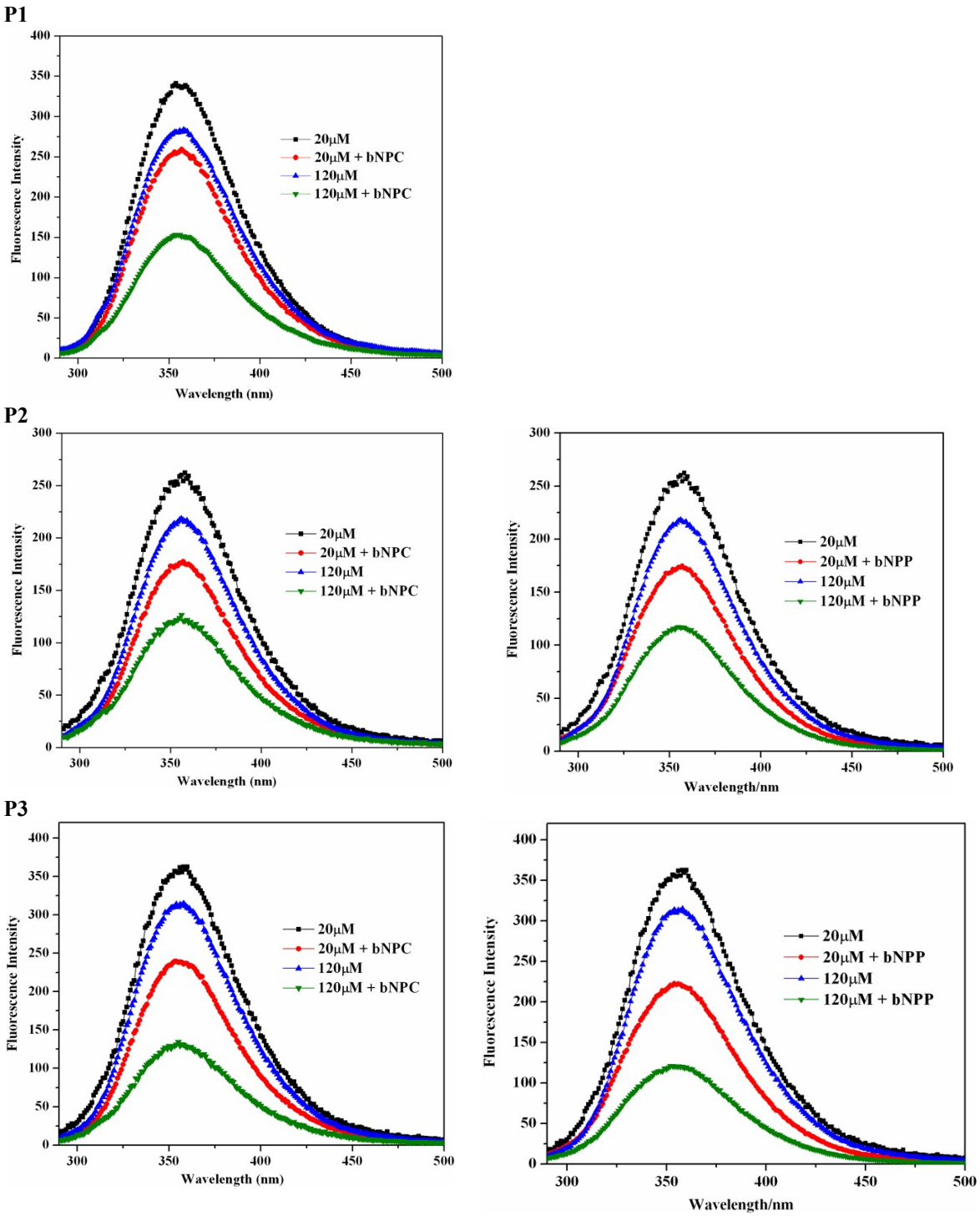


Figure S11: Fluorescence emission spectra at 298 K of peptides at 20 and 120 μM concentrations in absence and presence of the ligand in 100 μM concentration.

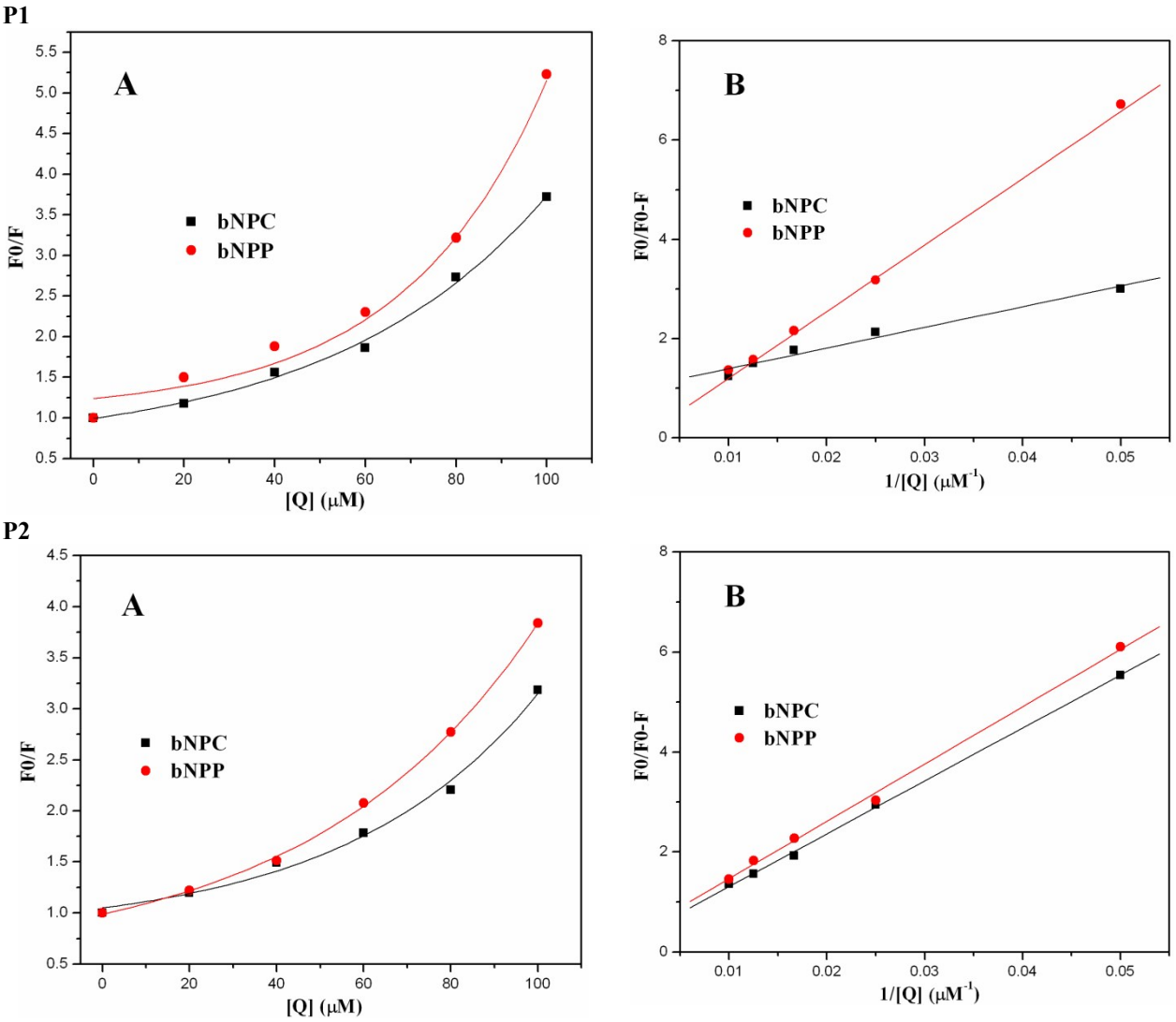


Figure S12: Plots of fluorescence quenching data for **P1** and **P2** at 120μM concentration with the ligands according to Stern-Volmer equation (left panel) and modified form of the equation as given in the Materials and Methods Section (right panel).