RX and XD ROESY peaks confirmed that the overall main chain conformation of the peptide is not folded.

4.5 Summary and Conclusions

The present work have described and compared the conformational preferences of Ac-RGD and Ac-RXD peptides in membrane mimicking solvents. MD simulations and experimental NMR results provide evidence for the unique conformational features of Ac-rGd, than the other analogs. This peptide experiences a folded conformation in both the solvents and stabilized by Arg-$N^{\varepsilon}H\cdots O{=}C^{\gamma}$-Asp hydrogen bonding interaction in DMSO-d_6. The prevalence of hydrogen bonding interactions have been validated from the NMR temperature coefficients experiments. To enhance our understanding of the structure and function of RGD analogs we have introduced another torsion angle μ between ϕ and ψ by incorporating β-Ala residue in between Arg and Gly, both MD simulation and NMR results suggest that though we have been able to enhance the activity than the Ac-rGD and Ac-RGd, it could not achieve the same conformational features as that of Ac-rGD and Ac-RGD. From these results we conclude that Ac-rGd is a better integrin binding analog than the native peptide Ac-RGD by changing the chirality of both chiral residues and we also infer another conclusion that introduction of β-Ala in various bioactive compounds instead of Gly or any structural similar compound may unravel unique conformational features and thereby its activity.