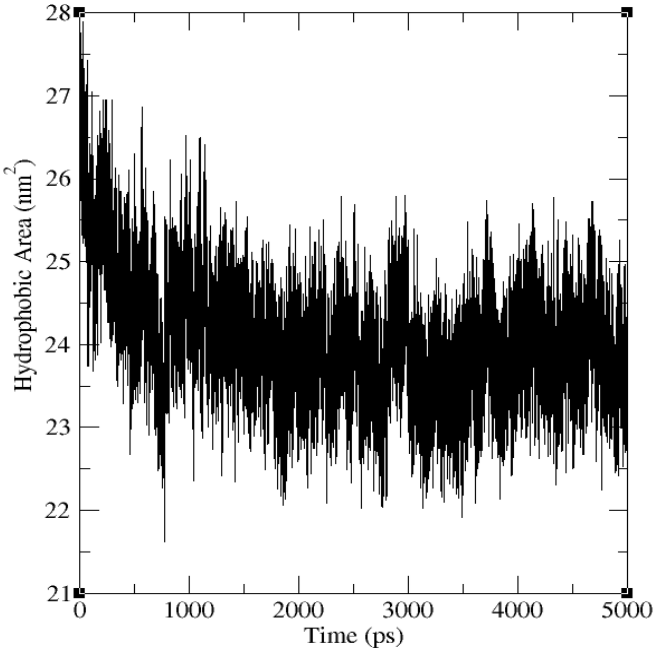
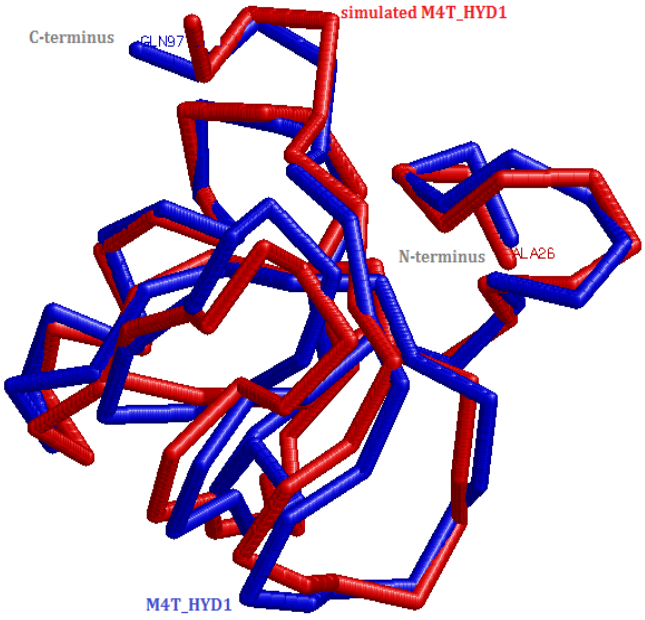


Figure 13: Hydrophobicity measurement as a function of time during simulation of M4T_HYD1

3.3.3 Overall Conformation Analysis

When the solvated protein now in dynamic form is analyzed against the original M4T_HYD1 protein, the conformation shows an RMSD value score of 0.291738 nm. Again the deviation lies in the acceptable range and can be credited to the secondary structure changes observed by DSSP (Table 2).



Figuer 14: Superimposed backbone structures of original and simulated HYD1 protein

Comparison of these two structurally aligned proteins with DSSP reveals that as HYD1 conformed to a less compact structure, there were significant loss of beta sheets, and less of the helix to other secondary structure elements like bends, hydrogen bond turns and amino acids not in atom records:

Table 2: DSSP three state composition of HYD1

	DSSP value (%)	
Method	M4T_HYD1	Simulated HYD1
Helix	15.3	13.9
Sheet	37.5	23.6
Others	47.2	62.5

However, the total content of sheet against that of helix in the secondary structure of the simulated protein still remains greater by approximately double that of helix. This can prove the theoretical fact that class hydrophobins attain a beta state in a water solvent.

4. Conclusion and Future Scope

MD simulations were used to compute atomic trajectories by solving equations of motion numerically using the GROMOS96 43a1 empirical force field. From a dynamic point of view the HYD1 protein proved to be thermally stable in the presence of an explicit water environment at 298K and constant pressure conditions. The protein also attained a compact structure which was credited to the low energy fluctuating beta strands. These findings are in agreement with previous theoretical and experimental evidence on dynamics of class I hydrophobins in related filamentous fungi. The authors therefore look forward to use the simulated M4T_HYD1 structure for docking studies in pursuit of a potential inhibitor molecule against G. moniliformis.

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References

[1] H. A. B. Wosten, “Hydrophobins, the fungal coat unraveled”, Biochimica et Biophysica Acta 1469, pp.79-86, 2000.

[2] J. G. Wessels, J. G., “Hydrophobins: proteins that change the nature of the fungal surface”, Adv Microb Physiol. 38, pp.1-45, 1997.

[3] M. Stubner, G. Lutterschmid, R. F. Vogel, and L. Niessen, “Heterologous expression of the hydrophobin FcHyd5p from Fusarium culmorun in pastoris and evaluation of its surface activity and contribution to gushing of carbonated beverages”, Int. J. Food Microbiol. 141, pp.110-115, 2010.

[4] N. J. Talbot, M. J. Kershaw, E. G. Wakley, O. De Vries, and J. Wessels, “MPG1 Encodes a fungal hydrophobin involved in surface interactions during infection-related development of Magnaporthe grisea”, Plant Cell 8, pp.985-999, 1996.

[5] B. M. Linder, “Hydrophobins: proteins that self assemble at interfaces”, Curr. Opin. Colloid Interface Sci. 14, pp.356-363, 2009.

[6] X. Wang, H. P. Permentier, R. Rink, J. Kruijtzer, R. M. Liskamp, H. A. Wösten, B. Poolman, and G. T. Robillard, “Probing the self-assembly and the

accompanying structural changes of hydrophobin SC3 on a hydrophobic surface by mass spectrometry", Biophys J Vol.87, pp.1919-28, 2004.
[7] J. Bayry, V. Aimanianda, I. Guijarro, M. Sunde, and J. P. Latge, "Hydrophobins—Unique Fungal Proteins", PLoS Pathog Vol.8 Issue 5, e1002700, 2012.
[8] S. Askolin, M. Linder, K. Scholtmeijer, M. Tenkanen, M. Penttilä, M. L. de Vocht, H. A. Wösten, "Interaction and comparison of a class I hydrophobin from Schizophyllum commune and class II hydrophobins from Trichoderma reesei", Biomacromolecules Vol.7, pp.1295-301, 2006.
[9] C. W. Bacon, I. E. Yates, W. P. Norred, and J. F. Leslie, "Production of fusaric acid by Fusarium species", Applied and Environmental Microbiology Vol.62, pp.41, 39-41, 43, 1996.
[10] C. Mawere., S. Kumar. G, and S. Muzondo, "Comparative Modelling, Quality Assessment and Validation of HYD1", International Journal of Innovative Research in Computer and Comm. Eng, IV (5), pp. 4242-4250, 2014.
[11] B. Hess and C. Kutzner and D. van der Spoel and E. Lindahl, "GROMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation ", J. Chem. Theory Comput. 4 pp. 435-447, 2008.
[12] W. Kabsch, and C. Sander, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features," Biopolymers 22 (12) pp. 2577-637, 1983.
[13] R. Sayle and E. J. Milner-White. "RasMol: Bimolecular graphics for all", Trends in Biochemical Sciences (TIBS), 20 (9), p. 374, 1995.
[14] The PyMOL Molecular Graphics System, Version 1.5.0.4, Schrödinger, LLC. [Online]. Available: http://www.pymol.org/
[15] R. C. Rizzo, "MD Simulation: Protein in Water", para. 13, Aug. 15, 2013. [Online]. Available: http://ringo.ams.sunysb.edu/index.php/MD_Simulation:_Protein_in_Water_Pt2. [Accessed: Aug. 1, 2014].

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