Protein structure in the gas phase

David van der Spoel
Dept. of Cell and Molec. Biol., Uppsala University

The gas-phase provides a hostile environment for biological specimens, like proteins. Nevertheless mass spectrometry routinely probes proteins and peptides outside their native environment. In order to facilitate and strengthen interpretation of such experiments we provide a structural underpinning based on simulations. We find in general that solution structures of proteins are largely maintained upon complete dehydration [1,2]. Encapsulation of proteins inside thin water layers or lipds or detergent micelles further stabilizes the native structure [3,4].

[1] A. Patriksson, E. Marklund and D. van der Spoel, Biochemistry 46 (2007) 933 [2] E. Marklund, D.S.D. Larsson, A Patriksson, D. van der Spoel and C. Caleman, Phys. Chem. Chem. Phys. 11 (2009) 8069 [3] Y. Wang, D.S.D. Larsson and D. van der Spoel, Biochemistry 48 (2009) 1006 [4] R. Friemann, D.S.D. Larsson, Y. Wang and D. van der Spoel, J. Amer. Chem. Soc. 131 (2009) 16606