# Shape and compactness of proteins studied by a combined NMR - SAXS approach

Using liquid-phase 1H NMR measurements we determined the diffusion coefficients and the apparent hydrodynamic radii (RH) of proteins and protein – lipid associates. Under the same experimental conditions the gyration radii (RG) were deduced from the initial region of the small angle X-ray scattering (SAXS) curves. We have studied the effect of concentration, temperature and ionic strengths on these characteristic values to describe the changes of the shape-factor defined by the RG/RH ratio.

We investigated the apo- and Ca2+ bound forms of calmodulin and showed that there is only a minor difference between their radius of gyration, and no variation in the apparent hydrodynamic radius, even though a conformational change occurs.

We also showed that DHPC micelles have an elongated shape and studied temperature, ionic strength and buffer type dependent changes in size and shape for the neutral and negatively charged bicelles (DHPC/DMPC, and DHPC/DMPC/DMPG). Moreover, we investigated the changes occurring in the presence of a model transmembrane peptide (KALP23) and of a surface-active peptide (melittin). Based on the scattering patterns we performed both size and shape determination of bicelles.

In conclusion, we proved that the shape factor determination is a useful and reliable parameter for characterization of protein compactness.