**Characterization of molecular shape and compactness by NMR-SAXS approach**

Using 1H NMR measurements we defined diffusion coefficients from the intensity-gradient strength curves and calculated further the values of apparent hydrodynamic radius (RH). From the same sample under the same experimental conditions SAXS measurements were performed. The initial region of the scattering curve permitted calculation of the gyration radius (RG). First we investigated the concentration, ionic strengths and temperature dependence of RH and RG for the well -known globular lysozyme protein. We followed the variation of the RG/RH ratio, a number that can characterize molecular shape.

We validated our results on other systems as well. We studied the apo- and Ca2+ bound forms of calmodulin showing there is little difference in the radius of gyration, and none in the apparent hydrodynamic radius, even though a conformational change occurs. Our statements were supported by a recent publication as well (Panjkovich; Svergun: PhysChemChemPhys, 2016). We also showed that DHPC micelles have an elongated shape in accordance with literature data (Lin et al, JACS, 1986).

Concluding we proved and tested for several systems that the shape factor determination is a useful parameter in defining protein compactness.