Influence of Temperature and Surface Composition on the Protein Hydration Shell

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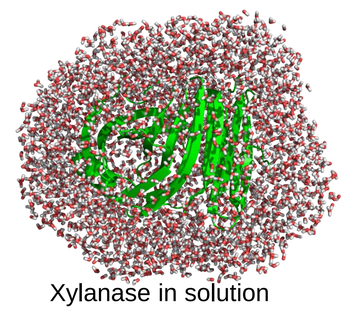
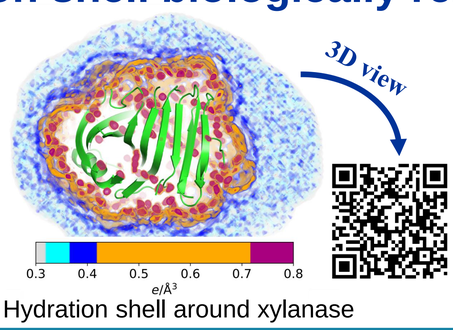
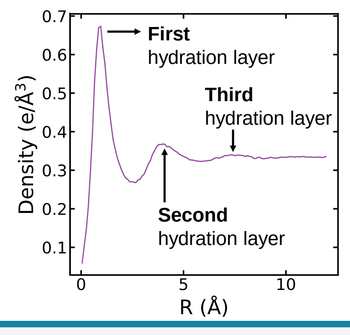
Why is the hydration shell biologically relevant?

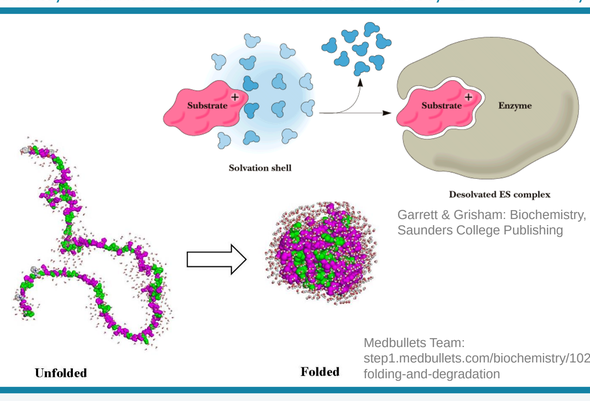


Xylanase in solution



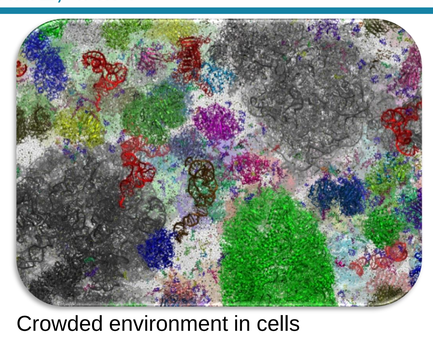
Hydration shell around xylanase





Garrett & Grisham: Biochemistry, 2/e, Fig. 16.5, Saunders College Publishing

Medbullets Team: step1.medbullets.com/biochemistry/102094/protein-folding-and-degradation

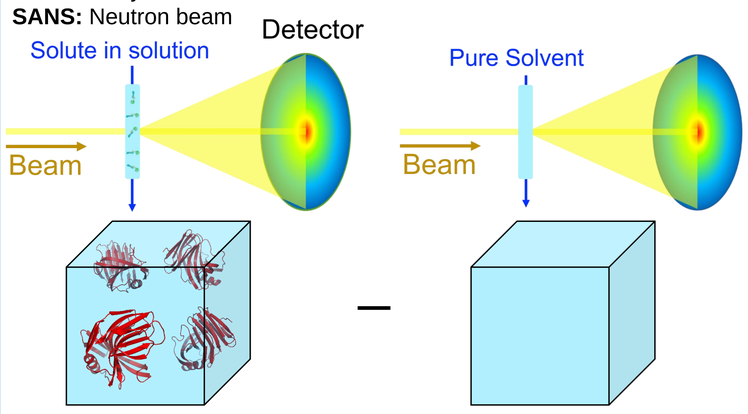


Crowded environment in cells
⇨ nearly all water is part of a protein hydration shell

Michael Feig et. al., *J. Mol. Graph.Model.* **2015** 58

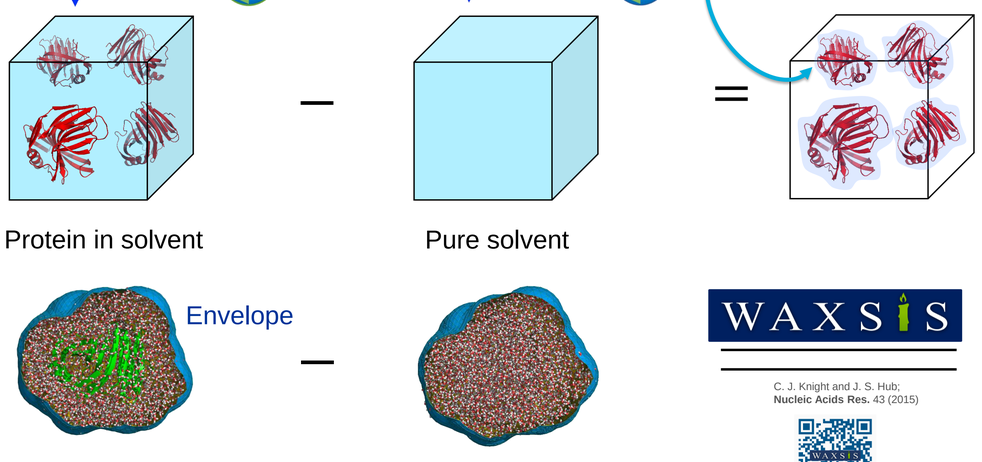
Small-angle scattering (SAS)

SAXS: X-ray beam
SANS: Neutron beam

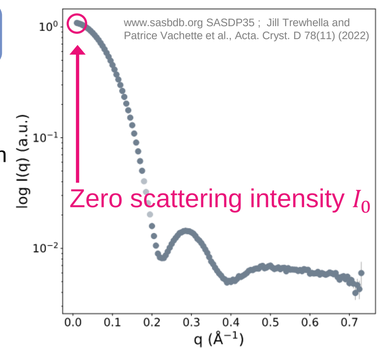


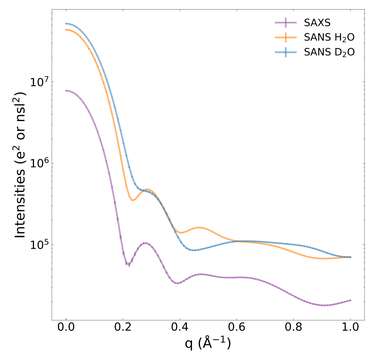
$$I_A(q) - I_B(q) = I(q)$$

Intensity of solution — Intensity of pure solvent — Scattering intensity



SAS provides information on the protein hydration shell



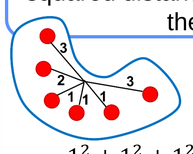


WAXSIS

C. J. Knight and J. S. Hub; **Nucleic Acids Res.** 43 (2015)

Radius of gyration R_g

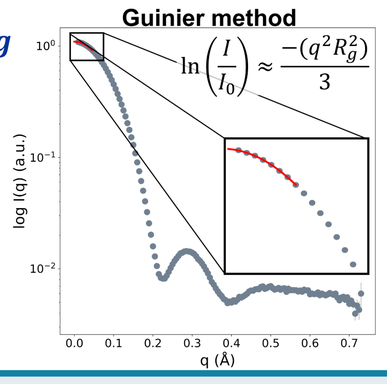
R_g^2 is the average density-weighted squared distance from the center of the object

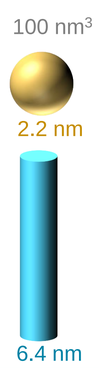


$$R_g^2 = \frac{\int r^2 \rho(r) dr}{\int \rho(r) dr}$$

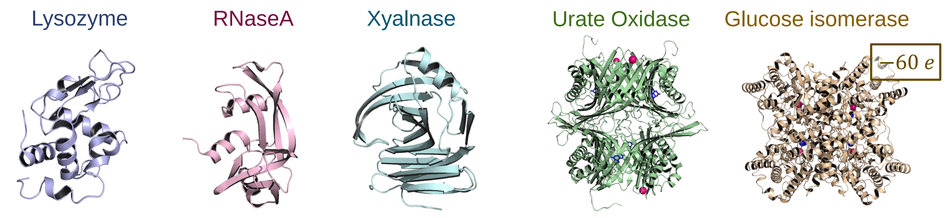
$$R_g^2 = \frac{1^2 + 1^2 + 1^2 + 2^2 + 3^2 + 3^2}{6} = 4.167$$

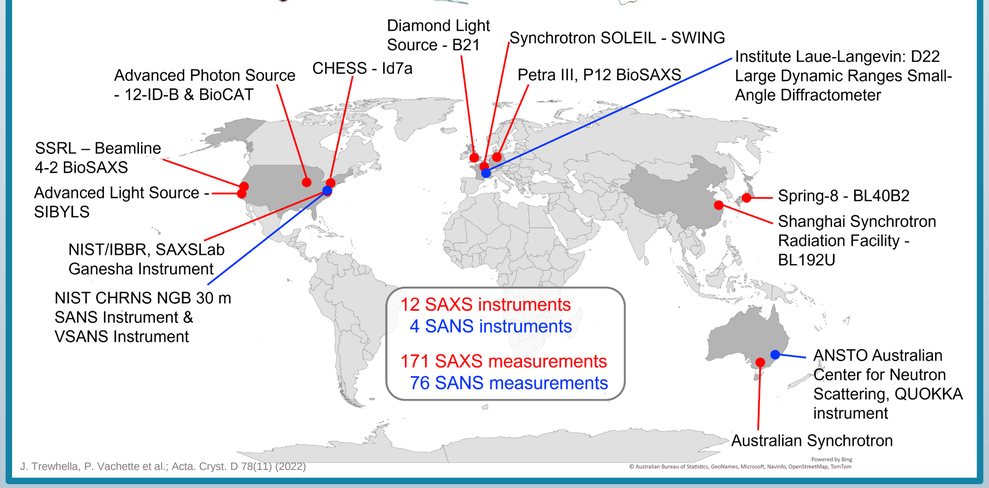
$$R_g = \sqrt{4.167} = 2.04124$$





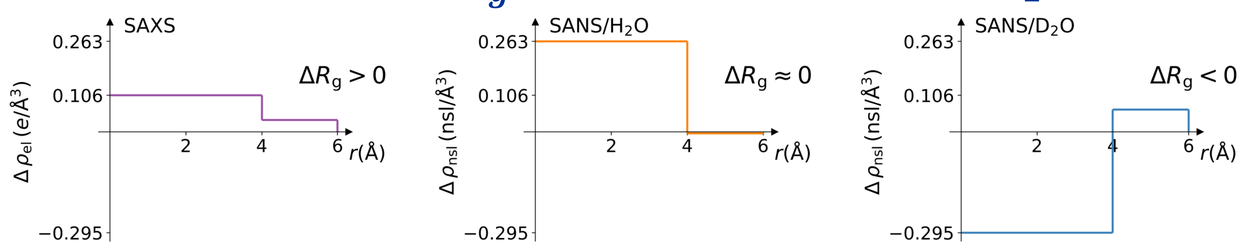
Worldwide round-robin benchmark





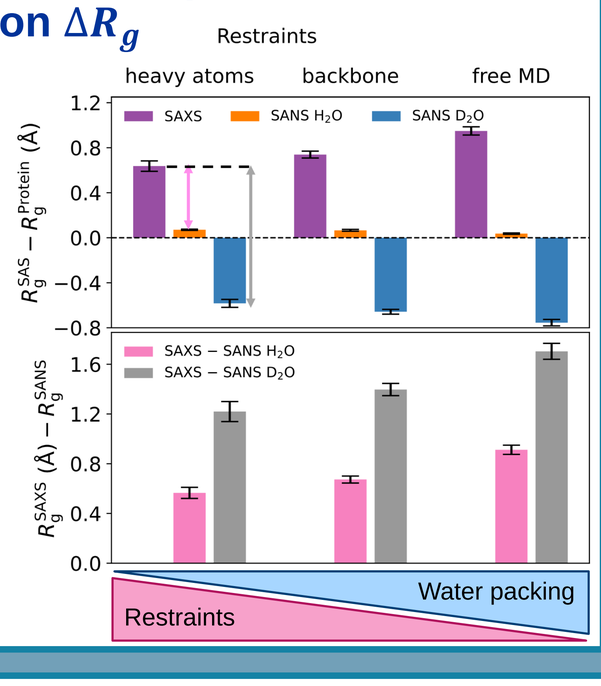
J. Trewhella, P. Vachette et al.; Acta. Cryst. D 78(11) (2022)

Hydration shell effect on R_g differs in SAXS, SANS/H_2O, SANS/D_2O

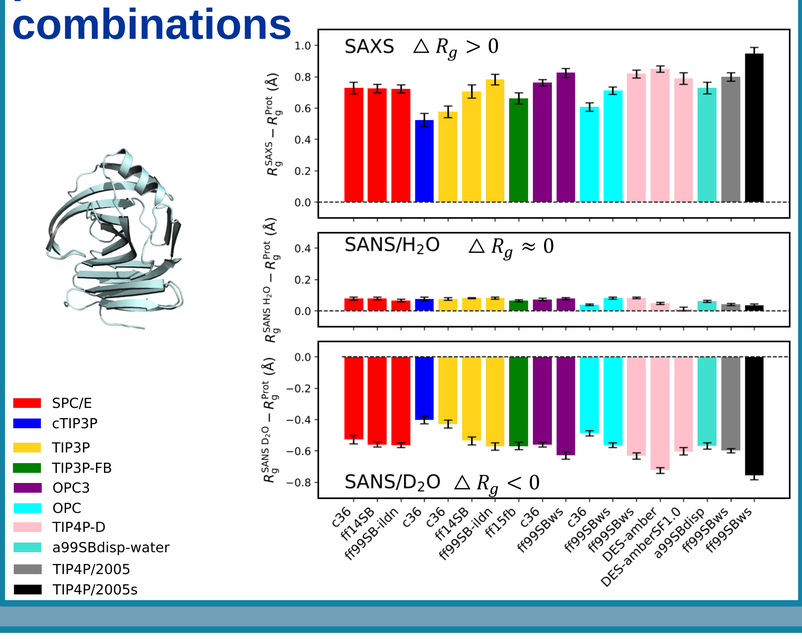


SAXS: R_g depends on the electron density (ρ_{el}) **SANS:** R_g depends on neutron scattering length density (ρ_{nsl})

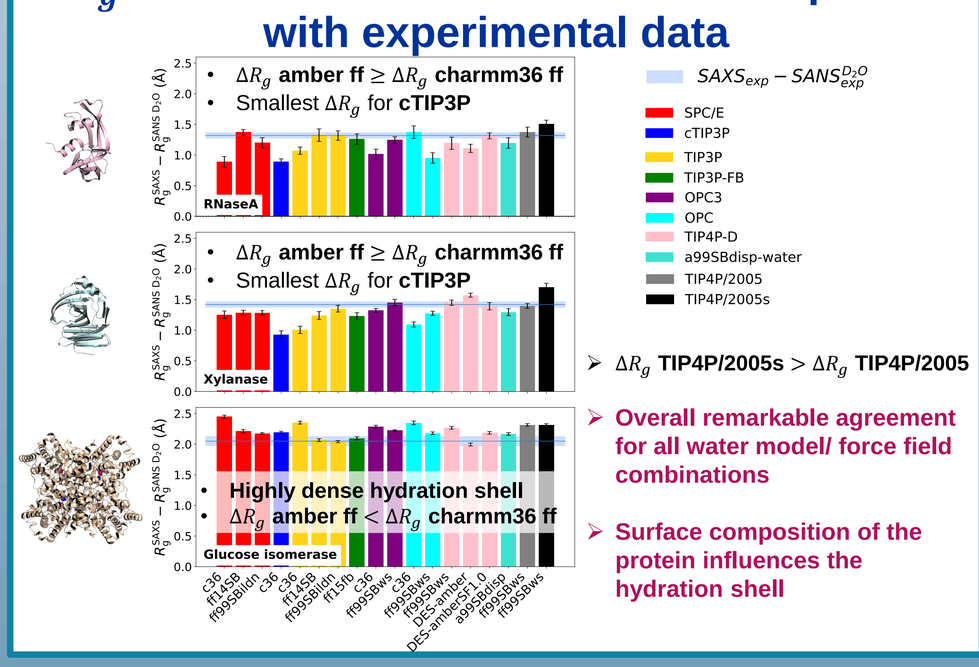
Effect of protein fluctuations on ΔR_g



Hydration shell effect on R_g from 18 protein and water force fields combinations



R_g from SAXS relative to SANS compared with experimental data



- ΔR_g **TIP4P/2005s** > ΔR_g **TIP4P/2005**
- **Overall remarkable agreement for all water model/ force field combinations**
- **Surface composition of the protein influences the hydration shell**

Unpublished data

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