Biomolecules on their way to solvation

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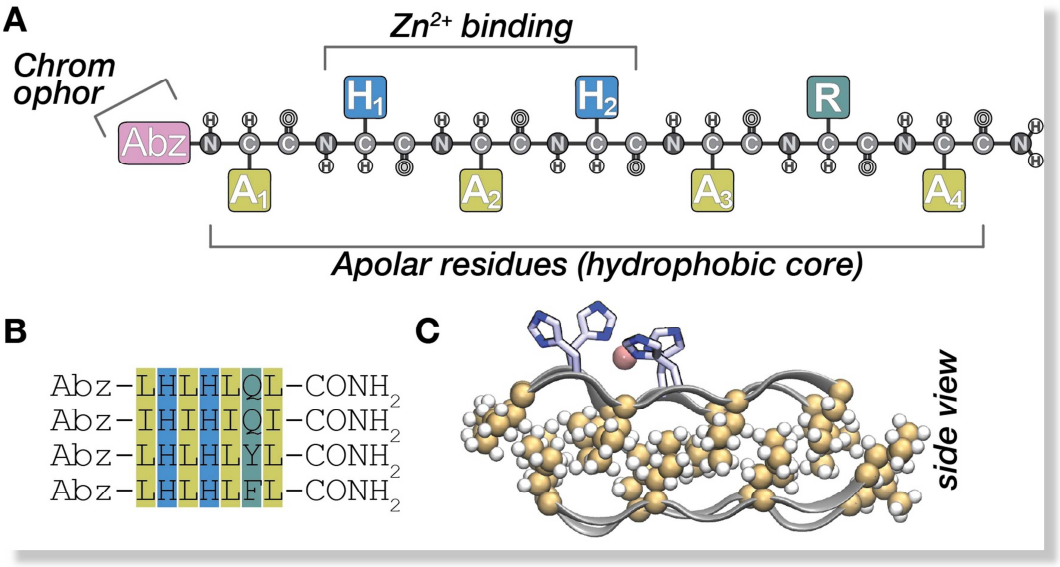

We investigate how the specific interactions that make-up solvation, i.e. interaction with water molecules and ions, shape biomolecules. We do so by a reductionist approach, starting with the bare molecular species in isolation and then adding in a stepwise manner more molecules of the same kind to understand oligomer formation, as well as investigating the effect of ions and water molecules on the oligomerization process. Experimentally we can realize these gas-phase clean-room conditions by employing mass-spectrometry based techniques. On the theory side we rely on molecular simulations that employ the first principles of density-functional theory (DFT).

Specifically, we will study a series of peptides (see A and B) that can form β-sheet aggregates (see C) and that can bind Zn^{2+} cations (see A and C). We will employ conformer selective spectroscopies like IR/UV double resonance or IR spectroscopy in combination with ion-mobility pre-selection of conformers. In addition we will perform DFT simulations of infinite assemblies of these peptides to study cooperativity of the interactions and also study oligomers of different size that are observed in the experiments.

<u>Further reading:</u>

- CM Rufo, YS Moroz, OV Moroz, J Stöhr, TA Smith, X Hu, WF DeGrado, IV Korendovych „Short peptides self-assemble to produce catalytic amyloids“ *Nature Chemistry* 6 (2014): 303-309.
- C Baldauf, K Pagel, S Warnke, G von Helden, B Koksch, V Blum, M Scheffler „How cations change peptide structure“ *Chem Eur J* 19 (2013): 11224-11234.
- S Warnke, C Baldauf, MT Bowers, K Pagel, G von Helden „Photodissociation of Conformer-Selected Ubiquitin Ions Reveals Site-Specific cis/trans Isomerization of Proline Peptide Bonds“ *J Am Chem Soc* 136 (2014): 10308-10314.
- TN Wassermann, O Boyarkine, B Paizs, TR Rizzo „Conformation-Specific Spectroscopy of Peptide Fragment Ions in a low-Temperature Ion Trap“ JASMS 23 (2012): 1029-1045.