Temperature-induced collapse of elastin-like peptides studied by 2DIR spectroscopy

O. Selig¹, F.C.M. Smits², M.B. van Eldijk², J.C.M. van Hest² and <u>Y.L.A. Rezus</u>¹*

¹FOM institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands ²Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 13, 6525 AJ Nijmegen, The Netherlands

*rezus@amolf.nl

We use 2DIR spectroscopy to study the conformational dynamics of elastin-like peptides in both their soluble and aggregated form. We find that the peptides remain surprisingly well hydrated in the aggregated state. In addition, we find evidence for the presence of an intramolecular hydrogen-bond in both states.

Elastin-like peptides (ELP) are thermo-responsive biopolymers which are soluble in water at low temperatures but undergo an inverse-temperature transition (ITT) upon heating. The transition involves the conformational collapse of the peptides, which leads to their aggregation. This temperature-induced transition makes ELPs interesting candidates for a wide range of applications, such as drug delivery, nano-assembly and chemical purification.

Here we use ultrafast 2DIR spectroscopy to study the molecular origin of the inverse temperature transition. To this end we probe the conformational fluctuations of elastin-like peptides of varying lengths. In particular, we focus on the vibrational energy transfer dynamics that occur within the amide I mode of the elastin-like peptides. We have compared these dynamics for a long ELP (450 residues) and a short ELP (5 residues). We find that only the long ELP shows the temperature-induced collapse. A very similar conformational transition can, however, be induced in the short ELP by replacing the aqueous solvent by trifluoroethanol (TFE). Interestingly, we find that the aggregation of the long ELP is not accompanied by significant dehydration of the peptide backbone. Moreover, we find evidence for the presence of an intramolecular hydrogen bond in both the long and the short ELP.



Fig.1 2DIR spectra of the amide I mode of a 450-residue elastin-like peptide for different pump-probe delays. The spectra in the upper panels are for a temperature below the aggregation temperature and those in the lower panels for a temperature above the aggregation temperature.