# Vienna-DNP:

# Methyl-based NMR methods for characterization of large peptide self-assemblies

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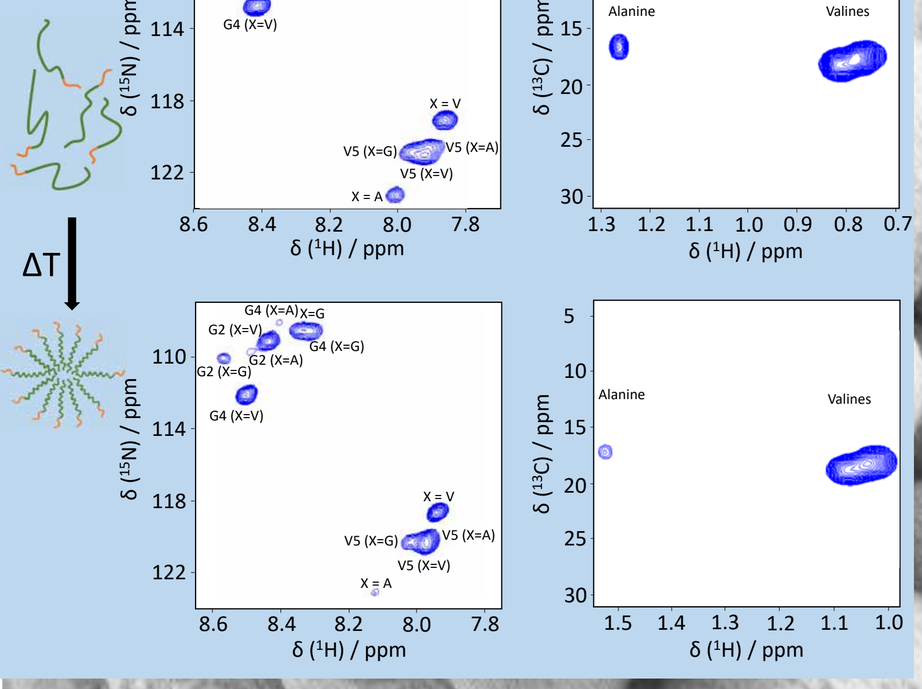
Nuclear Magnetic Resonance (NMR) spectroscopy is a key method for studying the structural dynamics of peptides and proteins in their native aqueous environment. However, due to weak signal intensities, in particular for high molecular weights, its application to peptide self-assemblies still needs to be improved. Our group previously described an NMR-based approach for real-time monitoring of assembly of the biomimetic R5 peptide,[1,] which forms supramolecular structures upon exposure to phosphate and co-precipitates upon silicate exposure.[2] Herein, we present a new approach utilizing methyl groups as intrinsic spin labels, with favorable relaxation properties resulting in improved sensitivity and a smaller sampling rate of 1 $min^{-1}$. This enables us to extend our approach to even bigger supramolecular assemblies of Elastin-like Polypeptide (ELP) – R5 fusion constructs, also providing a silica precipitation mechanism.[3]

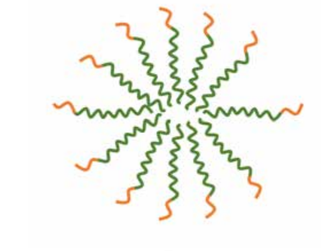
$[PGXGV]_{90}$ – ENLYFQ – GSSKKSGSYSGSKGSKRRIL

X = 27 × G, 18 × A, 44 × V

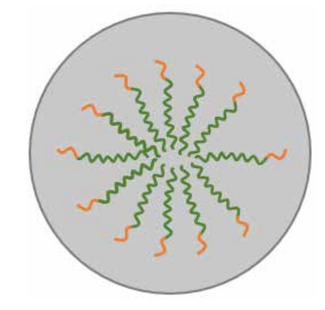








+ $Si(OH)_4$



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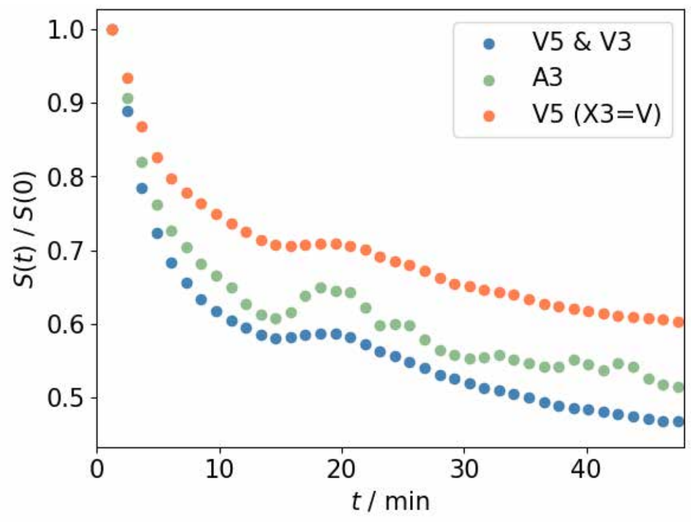
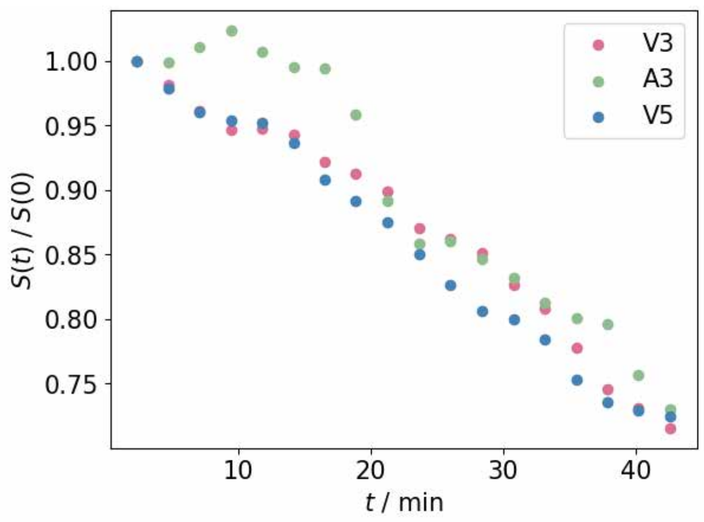
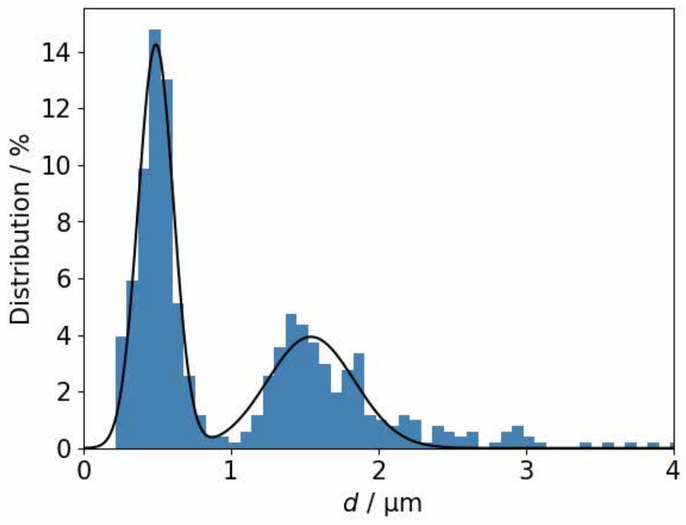
Real-time monitoring of silica precipitation process with methyl NMR.




Real-time monitoring of silica precipitation process with conventional backbone NMR.




Bimodal size distribution of Particles formed by ELP-R5.




## References:

[1] Strobl, J., Kozak, F., Kamalov, M., Reichinger, D., Kurzbach, D., Becker, CFW., Advanced Materials 2207586 (2023).
[2] Kozak, F., Brandis, D., Pötzl, C., Epasto, L. M., Reichinger, D., Obrist, D., Peterlik, H., Polyansky, A., Zagrovic, B., Daus, F., Geyer, A., Becker, C. F., Kurzbach, D., Adv. Sci. 2401239 (2024).
[3] Han, W., MacEwan, S. R., Chilkoti, A. & López, G. P. Nanoscale 7, 12038–12044 (2015).

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