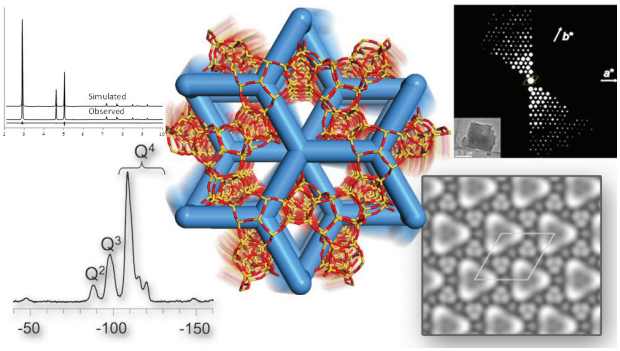

Figure 1. The structure of zeolite EMM-23 with the 3D channel system shown in blue (middle). The structure was solved by combining rotation electron diffraction (RED), HRTEM image, powder X-ray diffraction and solid state NMR.

Keywords: electron crystallography, electron diffraction, high resolution electron microscopy, crystallographic image processing, structure determination, space group determination, zeolite

MS11-O5 Structural insights into the conformation of the proline rich region of neuronal protein tau

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The Alzheimer's disease-associated protein tau is a typical representative of intrinsically disordered proteins (IDPs). Under physiological conditions, tau associates with microtubules and regulates their dynamics, whereas during the progression of neurodegeneration tau dissociates from microtubules, misfolds and deposits in brain tissue creating neurofibrillary tangles composed of paired helical filaments. The monoclonal antibody Tau5 was used as a surrogate tau protein binding partner to investigate the properties of the proline-rich region of tau molecule that contributes to its binding to microtubules. The Fab fragment of Tau5 has been crystallized alone and in complex with 30 amino acid long tau peptide ^{201}Gly-Arg^{230} [1] and both structures were solved to the 1.6 Å resolution [2]. The complex structure reveals the conformation of 16 residues long tau fragment and the comparison of both structures enables to observe the changes in the antibody paratope that occurred after binding of tau peptide. The kinetics of tau peptide binding to the tau5 Fab fragment was studied by the surface plasmon resonance analysis together with the evaluation of the impact of tau phosphorylation on sites T212, T217, T220 on the binding of tau peptide to the antibody. The molecular dynamics simulation was employed to evaluate the stability of the peptide conformation and the effects of phosphorylation. *Acknowledgement: This work was supported by the Slovak Research and Development Agency under the contract Nos. LPP-0038-09, APVV-0677-12 and by VEGA No. 2/0163/13.*

1. Cehlar, O.; Skrabana, R.; Kovac, A.; Kovacech, B.; Novak, M., Crystallization and preliminary X-ray diffraction analysis of tau protein microtubule-binding motifs in complex with Tau5 and DC25 antibody Fab fragments. *Acta Crystallogr F* **2012,** *68*, 1181-1185.

2. Cehlar, O.; Skrabana, R.; Dvorsky R.; Novak, M., Structure of tau peptide in complex with Tau5 antibody Fab fragment. *Acta Crystallogr D* (submitted 04/2015)

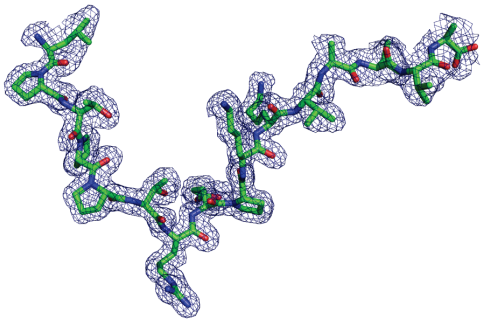

Figure 1. The structure of tau peptide ^{215}LPTPPTREPKKVAVVR^{230} with $2mF_O$-DF_C electron density contoured at the level of 0.5σ. The sidechain of R230 has not been modeled due to the lack of sufficient electron density

Keywords: intrinsically disordered proteins, protein tau, Fab fragment, peptide conformation

MS12. Crystallization and crystal treatment

Chairs: Terese Bergfors, Matthew Bowler

MS12-O1 Successful crystal formation - the journey from idea to fruition

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The availability of well-ordered crystals is essential to structure determination by X-ray crystallography. Nucleation is the first step that determines the crystallization process hence a search for the ultimate nucleating agent (nucleant) is ongoing. An ideal nucleant should induce efficient heterogeneous nucleation of crystals in a controlled manner and be effective in finding new crystallization condition and in improving crystal quality. It should be stable, easy to handle, and readily dispensed by robotics into numerous crystallization nano-droplets. This talk will discuss the strategies and the research of several years [1-4] resulting in our latest results [5] of the design, fabrication and validation of the first non-protein nucleating agents that can be used for the automated screening and optimization of any bio-macromolecule. These nucleants are dispensed using commercially available robots and their utilization bypasses the concerns associated with seeding, solid and viscous heterogeneous nucleants. The application of these materials is simple, quick, and 20 nanolitres is sufficient for each trial, thereby providing a potent tool for scientists in academia and industry endevouring to increase their success. References [1] Chayen *et al.* (2001) *J. Molecular Biology* **312**, 591-595 [2] Chayen, N.E. *et al.* (2006) *Proc. Natl. Acad. Sci. U. S. A.* 103, 597-601 [3] Saridakis et al (2011) *Proc. Natl. Acad. Sci. U. S. A.* 108, 11081-11086 [4] Khurshid *et al* (2014) *Nature Protocols 9,Pages:* 1621–1633 [5] Khurshid *et al.* (2015) *Acta Crystallographica* D **71**, 534-540. http://www.iucr.org/news/research-news/smart-crystallization http://www.imperialinnovations.co.uk/CRMIP

Keywords: crystallization, nucleation, proteins, macromolecules, automation, robotics