

Neutron Macromolecular Crystallography Workshop at ECM31

Where: [ECM31 venue](#) When: from 14h 21st August 2018, to 17h 22nd August 2018

Date/time	Speaker	Title
21st August		
Chair: John Helliwell		
14.00-14.30	Matthew Blakeley (ILL, France)	Neutron macromolecular crystallography: opportunities and challenges
14.30-15.00	Derek Logan (Lund, Sweden)	Analysis of protein, ligand and water hydrogen bonding in galectin-3 by neutron crystallography to guide drug design
15.00-15.30	Juliette Devos (ILL, France)	Deuteration of macromolecules and applications to neutron structural biology
15.30-16.00	Motoyasu Adachi (QST, Japan)	First neutron structural analysis of human casein kinase II
16.00-16.30	Tea/coffee	
Chair: Zoë Fisher		
16.30-17.00	Monika Spano (IBS, France)	Optimisation of crystal growth for neutron macromolecular crystallography
17.00-17.30	Katarina Koruza (Lund, Sweden)	How sweet to 'see' hydrogen atoms with neutrons: An explanation for carbonic anhydrase IX selective inhibition by saccharin and a derivative
17.30-18.30	Pavel Afonine (LBL, USA)	Phenix tools for neutron crystallography: from refinement to validation
22nd August		
Chair: Matthew Blakeley		
09.00-09.30	Tobias Schrader (JCNS, Germany)	Neutron protein crystallography at the Heinz Maier-Leibnitz Zentrum (MLZ): Is there anything to offer beyond neutrons?
09.30-10.00	José Gavira (CSIR-UGR, Spain)	Growing big from counter-diffusion techniques: gels and capillaries
10.00-10.30	Andrey Kovalevsky (ORNL, USA)	Unexpected protonation states and hydrogen bonding revealed by neutron crystallography in enzymes and nucleic acids
10.30-11.00	Tea/coffee	
Chair: Tobias Schrader		
11.00-11.30	Irene Schaffner (Vienna, Austria)	Combining X-ray/neutron crystallography to investigate structure-function relationships of chlorite dismutase
11.30-12.00	Ashley Jordan (ILL, France)	Magnetically aligned protein microcrystals for neutron diffraction studies
12.00-12.30	Flora Meilleur (ORNL, USA)	Neutron macromolecular crystallography to elucidate the mechanisms of industrial and biomedical enzymes
12.30-13.00	Andreas Heine (Marburg, Germany)	Ligand protonation and changes of the water inventory determined by high-resolution neutron structures upon trypsin complex formation
13.00-14.30	Lunch	
Chair: Matthew Blakeley		
14.30-15.00	Zoë Fisher (ESS, Sweden)	DEMAX: Deuteration and Macromolecular Crystallization Support labs for the European Spallation Source
15.00-15.30	Peter Moody (Leicester, UK)	The secrets of heme peroxidases uncovered by neutron crystallography
15.30-16.00	Marvin Seibert (Uppsala, Sweden)	Neutron crystallography of the carbon dioxide fixing enzyme Rubisco
16.00-16.30	John Helliwell (Manchester, UK)	Perspectives in neutron macromolecular crystallography
16.30-17.00	Discussion & closing remarks	