

Tuesday, 22nd April 2014

- 11:30 Coaches depart Coolangatta and Brisbane airports
- 13:00 Registration opens at Lost World Conference Centre (LWCC)
(All sessions at LWCC unless otherwise specified)
- 14:00 Light lunch LWCC
- 14:30-14:40 **Welcome and Opening Remarks**
Bostjan Kobe, UQ, SCANZ President

Session 1: Keynote 1

Chair: Mark Spackman, UWA

- 14:40-15:10 *Joanne Etheridge, Monash University*
Solving nanoscale structures using focussed electron beams

Session 2: Beyond Structure 1

Chair: Geoff Jameson, Massey

- 15:10-15:30 *Invited: Paul Low, UWA* – Twists and turns: the lessons hidden in disorder
- 15:30-15:50 *Invited: Juliet Gerrard, Canterbury U* – Protein nanotechnology: approaches to generating useful nanomaterials using protein tectons
- 15:50-16:10 *Invited: Helen Maynard-Casely, ANSTO* – Beyond structure with a WOMBAT, applications of neutron powder diffraction to planetary science.
- 16:10-16:30 *Invited: Danny Hatters, U Melbourne* – Biosensors to probe the nexus between protein conformations and cell functionality
- 16:30-18:30 **Sunset drinks at Moonlight Crag**
- 18:30-20:00 **Welcome Dinner (LWCC)**
including O'Reillys family history, animal encounter
- 20:00-21:30 **IYCr “Crystallography in Everyday Life” Photo Exhibit**

Wednesday, 23rd April 2014

Session 3: Mathieson Medal Lecture

Chair: Alice Vrielink, UWA

08:45-09:30 Medal Presentation and Lecture

Session 4: Keynote 2

Chair: Jack Clegg, UQ

9:30-10:00 *Andrew Goodwin, Oxford U*
Crystallography without crystals: Order within disorder

10:00-10.30 **Coffee/Tea and Exhibitor/Posters**

Session 5

Hot Structures in Biology

Chair: Joel Tyndall, Otago

10:30 *Invited: Bostjan Kobe, UQ*
Spring-hammer mechanism of metal ion binding and release by the *Streptococcus pneumoniae* substrate-binding protein PsaA

10:50 *Invited: Peter Czabotar, WEHI*
Structural insights into cell death

11:10 *Selected: Sandro Ataide, USyd*
The signal recognition particle RNA and its multi functions

11:25 *Selected: Nyssa Drinkwater, King's College London and Monash U*
Exploring the conformational flexibility of human IgE with a inhibitory Fab fragment

11:40 *Selected: Mary Christie, MPI Tübingen Germany*
Insights into the recruitment of the PAN2-PAN3 deadenylase complex to miRNA targets by the GW182/TNRC6 proteins

11:55 *Selected: Oleksiy Kovtun UQ*
Structural studies of the cavin proteins provide new insights into the mechanisms of caveolae formation

Session 6

Crystal Engineering

Chair: Stuart Batten, Monash

10:30 *Invited: Deanna D'Alessandro, USyd*
Exploiting redox-activity in metal-organic frameworks and porous coordination polymers for functional properties

10:50 *Invited: Jack Clegg, UQ*
Flexible crystals: stretching the boundaries of a single crystal

11:10 *Selected: Shane Kennedy, ANSTO*
The presence of mixed valence rare earths in RMn_2X_2 compounds

11:25 *Selected: Michael Pfrunder, QUT*
Halogen-bond mediated crystal engineering of metal complexes

11:40 *Selected: Natasha Sciortino, USyd*
Spin Crossover Induced Molecular Mosaic Patterning Generated in a 3D Porous MOF

11:55 *Selected: Sam Duyker, ANSTO*
Combined neutron scattering and DFT modelling studies of functional materials

12.10-13.30

Lunch Break and Exhibitor/Posters

Session 7: Beyond Structure 2

Chair: Suzanne Neville, U Sydney

- 13:30-13:50 *Invited: Jane Allison, Massey U*
Let the powers combine: hybrid methods in structural biology.
- 13:50:14:05 *Selected: Ming Wen Shi, UWA*
Reverse electrostatic complementarity based on the crystal structure of the pure protease inhibitor E64c
- 14:05-14:25 *Invited: Colin Jackson, ANU*
Crystal structures of ancestral amino acid binding proteins reveal protein specialization can occur through conformational selection
- 14:25-14:40 *Selected: Bhumika Shah, Macquarie*
Crystal structures of genomic island components from Australian *A. baumannii* strains
- 14:40-15:00 *Invited: Simon Grabowsky, UWA*
X-ray wavefunction refinement – introduction, examples, validation
- 15.00-15.30 **Coffee/Tea and Exhibitor/Posters**

Session 8: Materials and Metals

Chair: Alison Edwards, ANSTO

- 15:30-15:50 *Invited: Kate McGrath, McDermid NZ*
Using hydrogels to control crystallization: synthesizing next generation implant materials
- 15:50-16:10 *Invited: Neeraj Sharma UNSW*
Probing electrochemistry and crystal structure simultaneously
- 16:10-16:25 *Selected: Chris Ling, U Sydney*
First observation of intersite valence transitions involving $4d$ and $5d$ ions, as revealed by high-pressure X-ray and neutron diffraction
- 16:25-16:40 *Selected: Jay Bourke, Melbourne U*
Critical applications of high absolute accuracy XAFS measurements to low-energy inelastic electron scattering
- 16:40-16:55 *Selected: Kevin Jack, UQ*
Investigation and control of periodic microphases in composites of block copolymers and ionic liquids
- 17.00-18.30 **SCANZ Council Meeting (part I)**
- 18:30-19:30 **Pizza and Pasta Dinner sponsored by Bruker**
O'Reilly's Retreat Pavilion and Theatrette
- 20.00-22.00 **Poster Session (LWCC)**

Thursday, 24th April 2014

7:30-08:30 SCANZ Council Meeting (part II)

Session 9: Bragg Medal Lecture

Chair: Peter Colman, WEHI

08:45-09:30 Medal Presentation and Lecture

Session 10: Keynote 3

Chair: Jacqui Gulbis WEHI

9:30- 10:00 *Alice Vrielink, UWA*
Targetting multidrug resistance in Neisseria: A structural approach

10.00-10.30 **Coffee/Tea and Exhibitor/Posters**

Session 11: Drug Targets and Inhibitor Development

Chair: Helen Blanchard, Griffith U

10:30 *Invited: Begoña Heras, La Trobe U*
Structural diversity among autotransporter proteins

10:50 *Selected: Andreas Hofmann, Griffith*
Crystal structure and immunological properties of the first annexin from *Schistosoma mansoni*

11:05 *Selected: Genevieve Evans, Auckland*
The structure of a chorismate-utilizing enzyme from *Mycobacterium tuberculosis* supports the possibility of developing a “magic shot-gun” rather than a “magic bullet”

11:20 *Selected: Roisin McMahon, UQ*
Bacterial disarmament: DSB proteins as anti-virulence targets

11:35 *Selected: Khuchtumur Bum-Erdene, Griffith*
Design, development and validation of galectin-3-specific inhibitors

11:50-12:10 *Invited: Aaron Oakley, U Wollongong*
Tetrahydrocarbazoles: a future broad-spectrum antibiotic?

Session 12: Chemical Crystallography

Chair: Chris Howard, U Newcastle

10:30 *Invited: David Turner, Monash*
Laue neutron diffraction: Applications in chemical crystallography

10:50 *Selected: Suzanne Neville, USyd*
Targeting multi-step spin crossover in flexible coordination polymers

11:05 *Selected: Stuart Batten, Monash U*
Versatile nanoballs – multiple packings and multiple properties

11:20 *Selected: Alison Edwards, ANSTO*
Resolution, interpretation and modelling in chemical crystallography – critical analysis – furthering chemistry!

11:35 *Selected: Richard Welberry, ANU*
Local order in wüstite. Fe_{1-x}O , using a PDF approach

11:50-12:05 *Selected: Chris Chantler, UMel*
What will the new Volume of the International Tables for Crystallography be about? Volume I: XAS, Eds CT Chantler, B Bunker, F Boscherini

12.10-13.30 **Lunch Break and Exhibitor/Posters**

Session 13: Methods in Structural Biology

Chair: John Bruning, U Adelaide

- 13:30-13:50 *Invited: Airlie McCoy, Cambridge*
Fragment-based Molecular Replacement with Phaser
- 13:50-14:10 *Invited: Norelle Daly, JCU*
Structural insights into the role of the cyclic backbone in a squash trypsin inhibitor
- 14:10-14:25 *Selected: Alpeshkumar Malde, UQ*
Validation of ligands in X-ray crystal structures
- 14:25-14:40 *Selected: Anthony Duff, ANSTO*
The structure of the megadalton magnesium chelatase assembly
- 14:40-14:55 *Selected: Geoffrey Jameson, Massey*
First structure of a non-processive pectin methylesterase (from *Aspergillus niger*): comparison to processive orthologues from plants and bacteria

14.55-15.30 **Coffee/Tea and Exhibitor/Poster**

Session 14: Membrane Proteins

Chair: Simon Williams, UQ

- 15:30-15:50 *Invited: Hartmut Luecke, UC Irvine*
Structure, function, and inhibitors of the acid-gated *Helicobacter pylori* urea channel, an essential component for acid survival
- 15:50-16:05 *Selected: Joel Tyndall, Otago*
Structures of the full-length bitopic membrane protein CYP51 from *Saccharomyces cerevisiae* provide insight into substrate and drug binding and mutations affecting antifungal susceptibility
- 16:05-16:20 *Selected: David Aragao, Australian Synchrotron*
Crystal structure determination of the integral membrane diacylglycerol kinase
- 16:20-16:35 *Selected: Megan O'Mara, UQ*
A tale of three structures
- 16:35-16:50 *Selected: Julia Archbold, UQ*
Optimisation of G-protein coupled receptor expression and purification for structural studies

17.00-18.00 **SCANZ AGM**

19.30-10:00 **CONFERENCE DINNER** *sponsored by AXT/Rigaku/TTP*
O'Reilly's Mountain Café

Friday, 25th April 2014

Session 15: SCANZ 1987 Fund Plenary Lecture

Chair: Bostjan Kobe, UQ

08.40-09.30 *Petra Fromme, University of Arizona*
Membrane protein serial femtosecond crystallography using XFELs

09.30-10.00 **Coffee/Tea and Exhibitor**

Session 16: Rising Star Plenary Session

Chair: David Turner, Monash

10.00-10.15 *Jason Busby, Auckland*
The protein encapsulation and delivery mechanism of ABC toxins

10.15-10.30 *Josie Auckett, U Sydney*
The low-temperature magnetic anomaly of $\text{Ca}_2\text{Fe}_2\text{O}_5$ studied by single-crystal neutron diffraction

10.30-10.45 *Alastair Stewart, VCCRI*
The structure and dynamics of rotary ATPases

10.45-11.00 *Sophie Broughton, SVIMR*
New structural insights into receptor activation and assembly in the beta common cytokine family

11.00-11.15 *Thomas Ve, UQ*
Structural basis of disease resistance in flax against flax rust

11.15-11.30 *Sajesh Thomas, UWA*
Insights into vibrational stark effect from X-ray charge density analysis of supramolecular host-guest complexes

Session 17: Keynote 4

Chair: Jenny Martin, UQ

11:30-12:00 *Vic Arcus, Waikato University*
Crystallography and climate change: The temperature-dependence of biological rates

12:00-12:10 Closing Remarks and Handover to New President

12.10-12:50 Farewell Lunch

1.00 pm Coaches depart for airports

Wednesday 23rd April: Poster Session Presenters (* student poster)

- 1* **Bezerra**, Maria Júlia Barbosa: Federal University of Ceara Brazil “Vasorelaxant activity of *Canavalia grandiflora* seed lectin: A structural analysis”
- 2* **Blundell**, Ross: UQ “Characterisation of adenylosuccinate synthetase from the fungal pathogen *Cryptococcus neoformans*”
- 3 **Maynard-Casely**, Helen: ANSTO “Crystallography365 and Crystals in the City: IYCr 2014 activities”
- 4* **Brock**, Aidan J: U Queensland “Solvent exchange in a hierarchically assembled metal-organic framework”
- 5 **Bourke**, Jay D: U Melbourne “Density Functional Calculations of Electron Energy Loss Data and Inelastic Mean Free Paths in Elemental and Binary Materials”
- 6* **Brouwer**, Jason M: WEHI “Structural Insights into Bak Activation and Oligomerisation”
- 7 **Bruning**, John B: U Adelaide “Structural and Dynamic Studies of PPAR γ Agonism”
- 8* **Casey**, Lachlan W: UQ “In search of infinite solutions; the inverse problem in small-angle X-ray scattering”
- 9* **Chang**, Chiung-Wen: UQ “Structural basis of binding specificity between nuclear receptor: importin- α and non-classical nuclear localization signals”
- 10 **Chantler**, Chris T: U Melbourne “High accuracy calibration of a synchrotron X-ray beam using powder diffraction”
- 11* **Clairfeuille**, Thomas: UQ “The intersection of two central cellular trafficking pathways: the binding of SNX27 to the retromer complex”
- 12* **Cowan**, Angus D: WEHI “Structural Investigations into the Control of Pro-apoptotic Bcl-2 Family Proteins”
- 13* **Fellner**, M: Otago U “Implications of the cysteine-tyrosine crosslink in cysteine dioxygenase”
- 14 **Hall**, Syd: U Western Australia “Into the future with CIF: advances in data, metadata and meta-metadata applications”
- 15* **Horsefield**, Shane: UQ “Molecular basis of signaling by Toll/Interleukin-1 Receptor domain-containing adaptors in Toll-like Receptor pathways”
- 16 **Howard**, Christopher J: “Neutron study of the magnetic structures and phase transition in iron (III) phosphate, FePO₄”
- 17* **Jeon**, Yujung: UQ “Structural characterization of the mammalian CAD multienzyme complex”
- 18* **Lavrencic**, Peter: UQ “The functional and structural role of cysteine residues in Toll-like receptor signalling adaptor MAL/ TIRAP”
- 19* **Lawrence**, CF: WEHI “Structurally guided small molecule targeting of the Insulin and Type 1 Insulin-Like Growth Factor Receptors”
- 20 **Leneva**, Natalya; UQ “Structural characterisation of the retromer complex and associated sorting nexins”
- 21* **Luo**, Zhenyao: UQ “Structural elucidation of zinc acquisition mechanisms in *Streptococcus pneumoniae* and development of novel antibiotics against streptococcal diseases”
- 22* **Lv**, You; UQ “Phylogenetic mapping and structural comparison of bacterial ketol-acid reductoisomerase”
- 23* **Nematirad**, Melina: Monash U “Single molecule magnetism in μ -phenolato dinuclear lanthanide complexes containing heptadentate Schiff base ligand”
- 24 **Rae**, A David: ANU “Explicit and implicit data merging in crystallographic least squares”

25* **Roy**, Michael; WEHI “Elaboration of benzoylurea inhibitors targeting pro-survival Bcl-_{xL}”

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27* **Tabrizi**, Shabnam Tarahi; Macquarie U “Crystallization and Structure characterization of the Gun4 from *Chlamydomonas reinhardtii*”

28 **Tyndall**, Joel DA; U Otago “Multiple binding modes of isothiocyanate inhibitors of macrophage migration inhibitory factor define structure activity relationships”

29 **Walden**, Patricia M; UQ “A novel N-terminal domain may dictate the role of the disulfide bond protein α -DsbA2 from *Wolbachia pipientis*”

30 **Williams**, Simon “Disease resistance signaling in plant innate immune receptors, it’s all about dimerization”

31* **Wan**, Li; UQ “Crystal structure of a flax cytokinin oxidase and interaction studies with a fungal effector”

32* **Zhang**, Xiaoxiao; UQ “Plants vs. pathogens: structural and functional studies of Arabidopsis resistance protein SNC1 TIR domain and flax rust effector protein AvrP”