INSTITUTE FOR PROTEIN RESEARCH (OSAKA UNIVERSITY)
RESEARCH SCHOOL OF CHEMISTRY (AUSTRALIAN NATIONAL UNIVERSITY)
PROTEIN STRUCTURE AND FUNCTION
2nd JOINT SYMPOSIUM DECEMBER 3rd -5th 2017

KEYNOTE SPEAKERS

DAVID LAWSON
(Australia and Japan: Innovating for the Future)

HARUKI NAKAMURA
(Computational 3D Structure)

JOHN CARVER
(Crystallin Biology)

GENJI KURISU
(Photosynthetic Electron Transfer)

JUNICHI TAKAGI
(N-linked Glycans in Receptors)

THOMAS HUBER
(Protein Structure with Lanthanides)

MAL MCLEOD
(Analysis by Arylsulfatase Enzymes)

KIARAN KIRK
(Transporters as Antimalarial Targets)

KEYNOTE SPEAKERS

KYOSUKE NAGATA
(Changing Nature of Japan's Universities – 2017 and Beyond)

MARCO CASAROTTO
(Skeletal EC Coupling Machinery)

JOJI MIMA
(Rab-mediated Membrane Tethering)

HAFNA AHMED
(Mycobacterial Cofactor F420)

NOBUAKI OKUMURA
(Mechanism of Dipeptide Breakdown)

RICHARD CALLAGHAN
(P-glycoprotein Drug Binding)

JEN TAYLOR
(Proteomics in Emerging Cereal Crops)

JUNCHI HIGO
(Receptor Ligand Analysis *in silico*)

DAVID TREMETHICK
(Epigenetic Regulator H2A.B)

JOHN MANNERS
(Commercializing Ag-biotechnology)

TOSHIHIKO SUGIKI
(NMR of Lipid Transfer Protein)

JEREMY TAME
(Novel beta-Trefoil Lectins)

JOHANNES BUCHNER
(Molecular chaperones)

DAMIEN HALL
(A New Look at Protein Folding)

HIRONOBU HOJO
(Proteins from Chemical Synthesis)

LARA MALINS
(Late-Stage Peptide Modifications)

MAMORU TAKIZAWA
(Laminins and Integrins)

CHRISTOPH NITSCHE
(Reversible Covalent Modification)

KARMEN CONDIC-JURKIC
(Cloud Analysis of MD Simulations)

KAZUNARI IWAMOTO
(NFκB Super Enhancer Regulation)

STEVE SWAIN
(Genetic Regulation of Wheat Spikes)

VITTORIO BELLOTI
(Transthyretin Amyloidogenesis)

HIDEKI MOCHIZUKI
(Parkinson's Disease)

HIROTSUGU OGI
(Amyloid and Ultrasound)

YUJI GOTO
(Amyloid and Supersaturation)

CHRIS EASTON
(Radical Enzyme Biotechnology)

TOM MACPHERSON
(Dopamine D2L receptors)

KOHEI TAKESHITA
(Voltage-Gated Proton Channels)

Organizing Committee: John Carver, Yuji Goto, Masatomo So, Damien Hall and Haruki Nakamura.

Contact: Ms. Chizu Sasai Email: csasai@protein.osaka-u.ac.jp, Telephone: +81-6-6879-8614
Mr. Gavin Perri, Email: perri@rsc.anu.edu.au, Telephone: +61-2-6125-4401

Venue: Main Lecture Theater, Institute for Protein Research, Osaka University. ***Suita-campus, Osaka, Japan.***

Registration 9:00 am Sunday 3rd December

Welcome to the Second IPR/RSC Joint Symposium

(December 3rd-5th, 2017)

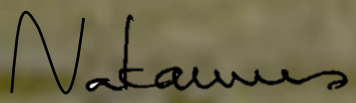
In 2015 the **Institute for Protein Research** (IPR) of Osaka University signed an institutional linkage agreement with the **Research School of Chemistry** (RSC) of the Australian National University. To mark this occasion a joint symposium with over fifty participants was held in Australia in November of 2015. To further cement the pairing of the two research institutes a second RSC-IPR joint symposium will be held in Osaka Japan, in early December, at the Institute for Protein Research.

The thematic cord of the three day event is '***Protein Structure and Function***'.

The Australian National University RSC website is http://chemistry.anu.edu.au/
The Osaka University IPR website is http://www.protein.osaka-u.ac.jp/en/

On behalf of the organizing committee I welcome you and truly hope that you have a wonderful and fruitful time in Japan.

Sincerely yours,



Haruki Nakamura, Professor
Director,
Institute for Protein Research,
Osaka University

Organizing Committee:

John Carver, Yuji Goto, Masatomo So, Damien Hall and Haruki Nakamura.

Administrative Liaison: Names and Telephone Numbers

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Mr. Gavin Perri
Email: perri@rsc.anu.edu.au
Telephone: +61 2 61254401

A Short History of Osaka University

Osaka University traces its origin back to 1869 when Osaka Prefectural Medical School was founded in downtown Osaka. The school later became the Osaka Prefectural Medical College with university status bestowed by imperial decree in 1919. The college merged with the newly founded College of Science to form Osaka Imperial University in 1931 and was inaugurated as the sixth imperial university in Japan. As part of the University, Osaka Technical College was later included to form the school of Engineering two years later. The university was eventually renamed Osaka University in 1947. Along with Tokyo and Kyoto Universities, Osaka University is currently considered as one of the top three universities in Japan.

A Short History of the Institute of Protein Chemistry at Osaka University

Osaka University had been active in the study of proteins and enzymes since its foundation in 1931, and it had been a long-standing desire of the University authorities to promote further this facet of the University's activities by establishing a research institute specialized in protein science. In 1955 an official plan was drafted to establish such an institute as a part of Osaka University and submitted to the Ministry of Education, Science and Culture. However, at the time the Ministry agreed to the opening of a new laboratory in the Faculty of Science for organic chemical studies of proteins and amino acids. The new laboratory was opened in 1956, and Professor Shiro Akabori, who had played a pivotal role in protein research at the Faculty of Science, was appointed as its supervisor. These early efforts helped to facilitate the establishment of a central institute for protein research, with the aim of facilitating close cooperation among researchers from a wide variety of scientific fields. In 1957, the Science Council of Japan urged the Government to consider the foundation of such an institute somewhere in the country. It was at this time that the Government decided to establish a research institute for protein science attached to Osaka University. The Institute for Protein Research (IPR) was thus founded formally on April 1, 1958, as a part of Osaka University, and Professor Shiro Akabori was appointed as its first director. The IPR began its research activities in an old building near the main building of the Faculty of Science at that time, which was located at Nakanoshima in downtown Osaka. Since then, protein research at IPR has made remarkable progress by elucidating structures and functions of proteins, and by understanding their biological roles from the molecular level to the cellular and the higher levels.

Through wide and strong support from the community, IPR has expanded over the last 55 years. Now, it has four divisions (16 labs) with an attached center, Research Center for State-of-the-Art Functional Protein Analysis (7 labs), which develops original techniques and applies them to reveal proteins' structure and function.

IPR has worked as an inter-university joint-use facility attached to Osaka University since its foundation. In April 2010, IPR was qualified as one of the Joint Usage/Research Centers in Japan by MEXT, Ministry of Education, Culture, Sports, Science and Technology. In particular, IPR offers the usages of its own synchrotron beam line at SPring-8 and of the Nuclear Magnetic Resonance (NMR) spectrometers with ultra-high sensitivities, to domestic and foreign protein researchers. In addition, IPR has constructed protein structural database (PDB: Protein Data Bank) as PDBj (PDB Japan), one of the four members of the wwPDB (worldwide PDB), which involves annotating the deposited data from structural biologists in Asian and Oceania region and by providing several original services and derived databases. PDBj-BMRB also constructs NMR experimental database, collaborating with BMRB (BioMagResBank) in U.S.A. IPR has also organized many international collaborative researches with foreign protein scientists.

Professorial and academic staff at the IPR (about 40 members) work hard at their own research, as well as for educational activities to undergraduate students at Faculty of Science and that of Medicine, and PhD. students at Graduate school of Science, Medicine, and Frontier Biosciences. From those Faculties and Graduate schools, approximately 100 students study at laboratories in IPR, and about 70 postdoctoral fellows make their own original investigations with various national and international research projects. Those students and postdoctoral fellows come from many different places in the world, and global human interactions are common at the IPR.

A Short History of the Australian National University

By the early 1870s Australia had three universities: the University of Sydney, founded 1850; the University of Melbourne, founded 1853; and the University of Adelaide, founded 1874. These universities were all founded under British traditions, with their primary aim being teaching. By 1900 there were calls made for the introduction of a National University of Australia that was to be primarily research focused.

In 1929 the Canberra University College (CUC), affiliated with the University of Melbourne, was established to provide undergraduate university education in Canberra, taking its first students in 1930. The CUC was integral in continuing to educate the influx of public servants to Canberra and for most of its history, students were part-time, sitting for University of Melbourne examinations and eventually graduating with a University of Melbourne qualification.

In 1946 the Australian Parliament passed the Australian National University Act 1946. The Act outlined the organization of ANU into two distinct groups: the Institute of Advanced Studies (IAS) and the Faculties. The IAS was to include institutes of medical science (later the John Curtin School of Medical Research), physical sciences, social sciences, Pacific studies and other fields of learning as the University Council determines. The establishment of the 'Faculties' did not take place until 1960 when the CUC (later the School of General Studies) was amalgamated with the IAS.

These efforts led to the establishment of the first four research schools at ANU: Research School of Physical Sciences (1947), the John Curtin School of Medical Research (1948); the Research School of Pacific Studies (1948) and the Research School of Social Sciences (1948). Expansion of the IAS continued with the establishment of the Research School of Biological Sciences (1967); the Research School of Chemistry (1968); the Centre for Resource and Environmental Studies (1973),the Research School of Earth Sciences (1973); the Research School of Astronomy and Astrophysics (1998), the School of Mathematical Sciences (1986-9) (now the Mathematical Sciences Institute), the Research School of Information Sciences and Engineering (1994); and the Research School of Humanities (2007).

A Short History of the Research School of Chemistry

The Research School of Chemistry (RSC) was founded in 1968. From the outset the School was concerned not only with in the results of pure research, but in providing a very advanced training ground appropriate to people, many of them from abroad, who would eventually work in other universities, in research institutions such as CSIRO, or in industry. Additionally, the fields of research originally selected were those of a fertile and developing nature and with foreseeable long-term interest in the Australian environment. Strong emphasis was placed on inorganic chemistry, on substances of biological interest (insect chemistry, antibiotic chemistry, plant chemistry), on synthetic chemistry which could be applied in many directions, and on aspect of solid-state chemistry and photochemistry. With its high level of instrumentation and the associated experts on its staff, RSC exerted a catalytic effect in making both instrumental services and experts available outside the School for research and teaching purposes.

The founding staff comprised two Professors, three Senior Fellows, five Fellows, eighteen Research Fellows and sixteen Scholars. The RSC now comprises over twenty research groups undertaking research across the breadth of the chemistry discipline. On 1st January 2009, the RSC merged with the undergraduate teaching facility, the Department of Chemistry, and the new Research School of Chemistry was born. Combining of the strengths of the two progenitors has resulted in a unique entity that offers the very best opportunities for studying chemistry at both the undergraduate and postgraduate levels.

In late 2013, the RSC entered a new era with its move from its four buildings into a new, large $90 million building with state-of-the-art laboratories, equipment and facilities. Adjacent to this research building is a purpose-built building that houses the laboratories for undergraduate practical classes. Both buildings are near the centre of campus and are co-located with the Research School of Biology in a science precinct. This new phase in the RSC's history help to ensure the School's continued output of world-leading research and teaching activities across a broad spectrum of chemistry areas.

Second RSC/IPR Joint Symposium (December 3rd-5th, 2017)

SPECIAL GUESTS

University of Tsukuba

Prof. Kyosuke Nagata: President of the University of Tsukuba.

Australian Government

Mr. David Lawson: Consul-General of Australian Consulate-General, Osaka.

Osaka University

Prof. Toru Fujiwara: Associate Executive Director, Global Engagement Office

University College London

Prof. Vittorio Belloti: Centre for Amyloidosis and Acute Phase Proteins

Technical University of Munich

Johannes Buchner: Department of Chemistry, Chair of Biotechnology

Yokohama City University

Prof. Jeremy Tame: Head of Drug Design Laboratory

ATTENDEES

Osaka University Institute for Protein Research

Prof. Haruki Nakamura

Prof. Genji Kurisu

Prof. Junichi Takagi

Prof. Hironobu Hojo

Prof. Yuji Goto

Prof. Junichi Higo

Assoc. Prof. Joji Mima

Assoc. Prof. Nobuaki Okumura

Assoc. Prof. Kohei Takeshita

Assoc. Prof. Damien Hall

Assist. Prof. Tom McPherson

Assist. Prof. Kazunari Iwamoto

Mr. Mamoru Takizawa

Osaka University, Graduate School of Engineering

Prof. Hirotsugu Ogi

Mr. Ryota Wakayama

Osaka University Medical School

Prof. Hideki Mochizuki

RSC Australian National University

Prof. John Carver

Prof. Thomas Huber

Prof. Chris Easton

Assoc. Prof. Mal Mcleod

Dr. Damien Hall

Dr. Lara Malins

Dr. Karmen Kondic-Jurkic

Dr. Hafna Ahmed

Dr. Christoph Nitsche

Mr. Thomas Loan

Mr. Hendrik Maat

Mrs. Elmira Bahraminejad

Mr. Ryota Wakayama

RSB Australian National University

Prof. Kiaran Kirk

Assoc. Prof. Richard Callaghan

JCSMR Australian National University

Prof. David Tremethick

Prof. Marco Casarotto

Mr. Spencer Richardson

Mr. Shouvik Aditya

Commonwealth Science and Industry Research Organization (CSIRO)

Prof. John Manners

Prof. Steve Swain

Dr. Jen Taylor

Symposium Program – Day 1

Sunday 3rd December (9am-6pm)	**12 talks (with 1 lunch break and 2 coffee breaks)**
9:00am- 10:00am	**Registration:** Institute for Protein Research Foyer
10:00am – 11:30am	**Session #1**
10:00 am - 10:30 pm (30minutes)	Consul-General David Lawson (Australian Consulate-General, Osaka)
10:30 am - 11:00 am (25minutes)	Prof. Haruki Nakamura (IPR)
11:00 am - 11:30 am (25minutes)	Prof. John Carver (RSC)
11:30am - 1:00pm	**Lunch (1 hour)**
1:00pm – 3:00pm	**Session #2**
1:00pm-1:30pm (25 minutes)	Prof. Genji Kurisu (IPR)
1:30pm-2:00pm (25minutes)	Prof. Thomas Huber (RSC)
2:00pm-2:30pm (25minutes)	Prof. Junichi Takagi (IPR)
2:30pm-3:00pm (25minutes)	Assoc. Prof. Mal Mcleod (RSC)
3:00pm - 3:15pm (15 minutes)	**Coffee**
3:15pm – 4:45pm	**Session #3**
3:15pm-3:45pm (25minutes)	Prof. Kiaran Kirk (Dean, ANU College of Science)
3:45pm-4:15pm (25minutes)	Prof. David Tremethick (Sub Director of JCSMR)
4:15pm-4:45pm (25minutes)	Prof. John Manners (Flagship Director- CSIRO)
4:45pm - 5:00pm (15 minutes)	**Coffee**
5:00pm – 6:00pm	**Session #4**
5:00pm-5:30pm (25minutes)	Assist. Prof. Toshihiko Sugiki (IPR)
5:30pm-6:00pm (25minutes)	Prof. Jeremy Tame (YNU)

6:10pm-6:30pm Transfer to dinner (25minutes)

Sunday 3rd Dinner (6:30pm-9:30pm): Dinner Event Restaurant TBD

6:30 pm	Seating at La Scena Restaurant (ラ・シェーナ) TEL: 06-6816-8411
7:20pm – 7:30 pm	Welcome and Introduction: Prof. Toru Fujiwara (Associate Executive Director, Global Engagement Office)
7:30pm – 8:30pm	Dinner Talk: Professor Kyosuke Nagata (President, University of Tsukuba)
9:30pm	Retire

Symposium Program – Day 2

Monday 4th December (8:30am-6pm)	**15 talks (with 1 lunch break and 2 coffee breaks)**
8:30am – 10:30am	**Session #5**
8:30am – 9:00 am (25 min)	Prof. Johannes Buchner (TMU)
9:00am -9:30 am (25 min)	Assoc. Prof. Damien Hall (IPR/RSC)
9:30am-10:00am (25min)	Prof. Hironobu Hojo (IPR)
10:00am-10:30am (25min)	Dr. Lara Malins (RSC)
10:30am -10:45am	**Coffee**
10:45am – 12:15pm	**Session #6**
10:45am-11:15am (20min)	Mr. Mamoru Takizawa (IPR)
11:15am-11:45am (25min)	Assoc. Prof. Marco Casarotto (JCSMR)
11:45am-12:15pm (25min)	Assoc. Prof. Nobuaki Okumura (IPR)
12:15pm-1:30pm	**Lunch (Catered) and Student Poster Display (Setup 9:00am)**
1:30pm – 3:30pm	**Session #7**
1:30pm-2:00pm (25min)	Assoc. Prof. Richard Callaghan (RSB)
2:00pm-2:30pm (25min)	Assoc. Prof. Joji Mima (IPR)
2:30pm-3:00pm (25min)	Dr. Jen Taylor (CSIRO)
3:00pm-3:30pm (25min)	Dr. Hafna Ahmed (RSC)
3:30pm-3:45pm	**Coffee**
3:45pm – 5:45pm	**Session #8**
3:45pm-4:15pm (25min)	Prof. Junichi Higo (IPR)
4:15pm-4:45pm (25min)	Dr. Karmen Condic-Jurkic (RSC)
4:45pm-5:15pm (25min)	Assist. Prof. Kazunari Iwamoto (IPR)
5:15pm-5:45pm (25min)	Prof. Steve Swain (CSIRO)

6:00pm-6:30pm Transfer to dinner (25minutes)

Monday 4th Dinner (6:30pm-9:30pm): Dinner Event Restaurant TBD

6:30 pm	Seating at Sakazuki Izakaya (和風バル) TEL: 050-3476-4575
7:30pm – 8:00pm	Dinner Talk: Professor Yuji Goto
9:30 pm	Retire

Symposium Program – Day 3

Tuesday 5th December (9:00am-12pm) 8 talks (with 1 coffee break)

8:30am – 10:30am	**Session #9**
8:30am -9:00am (25 min)	Prof. Vittorio Belloti (UCL)
9:00am -9:30am (25 min)	Prof. Hideki Mochizuki (Osaka Uni. Med.)
9:30am-10:00am (25min)	Prof. Hirotsugu Ogi (Osaka Univ. Eng.)
10:00am-10:30am (25min)	Prof. Yuji Goto (IPR)
10:30am - 10:45am	**Coffee**
10:45am – 12:45am	**Session #10**
10:45am – 11:15am (25min)	Prof. Chris Easton (RSC)
11:15am – 11:45am (25min)	Assist. Prof. Tom Macpherson (IPR)
11:45am-12:15pm (25min)	Dr. Christoph Nitsche (RSC)
12:15pm-12:45pm (25min)	Assist. Prof. Kohei Takeshita (IPR)
12:45pm-1:15pm (25min)	**Concluding Remarks: Prof. Nakamura and Prof. Carver**

SUNDAY 10:00 am- 10:30am

David Lawson

Email: David.Lawson@austrade.gov.au

Institution: Australian Consulate-General, Osaka
Australian Trade & Investment Commission

Position: Consul-General and Senior Trade Commissioner

Talk Title: Australia and Japan: Innovating for the Future

Abstract: 2017 is the 60th anniversary of the signing of the Australia Japan Commerce Treaty – enabling the start of Japan's investment into the sectors which have underpinned Australia's exports to Japan primarily in the resources and energy sectors. However, the nature of Australia's trade with Japan is now surprisingly sophisticated and last year Japan surpassed the UK to become the 2nd largest source of FDI in Australia. But what is happening in the sphere of science and technology and how are Japanese and Australians working together to enhance innovation and build the next generation of industries? Consul-General Lawson will talk about some of the trends in cross-border innovation paths between Australia and Japan. He is a graduate of the ANU and also has a Masters degree in Commercialisation of Science & Technology.

Web:

https://www.austrade.gov.au/Local-Sites/Japan

https://www.linkedin.com/in/davidlawson1

http://japan.embassy.gov.au/

SUNDAY 10:30 am- 11:00am

Haruki Nakamura

Email:

harukin@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: Director, Professor of Laboratory of Protein Informatics and Laboratory of Protein Databases

Talk Title:Integrative/Hybrid Structural Biology – Concept, Background, Tools, Data Archiving, Validation, and Future

Abstract: In recent years, the structures of very large macromolecular machines in cells have been determined by combining observations from multiple, complementary experimental methods, such as X-ray crystallography, NMR spectroscopy, 3DEM, small-angle scattering (SAS), FRET, crosslinking, and many others. Currently, many structures determined by such hybrid methods appear in high-impact-factor journals, and are being deposited in the PDB (Protein Data Bank), which is managed by an international organization, the wwPDB (worldwide PDB: https://wwpdb.org/), A new proto-type archive, PDB-Dev, has also just started (https://pdb-dev.wwpdb.org). Several issues for the new research field will be introduced and discussed.

Web:

http://www.protein.osaka-u.ac.jp/rcsfp/pi/

https://pdbj.org/

SUNDAY 11:00 am- 11:30am

John Carver

E-mail: john.carver@anu.edu.au

Institution: Research School of Chemistry,
Australian National University

Position: Director, Research School of Chemistry, Australian National University

Talk Title: Lens crystallin proteins, their post-translational modifications and cataract

Abstract: Crystallin proteins are the major component of the eye lens. In mammals, there are three types: α, β and γ. Crystallins are present at very high concentration and are arranged in a supramolecular order that ensures proper refraction of light and hence lens transparency. With age, extensive post-translational modifications (PTMs) occur to the crystallins which build up and contribute to lens opacification and cataract formation. Using a variety of protein chemical, biophysical and spectroscopic techniques, we have been examining the structural and functional changes that occur to individual crystallins as a result of PTMs such as deamidation (in particular, the conversion of asparagine to aspartic acid at selected sites), racemization (for example, conversion of L- to D-aspartic acid) and oxidation (disulphide bond formation). The consequences of these changes on the interactions of the crystallins will be discussed, and hence the relationship to cataract development.

Web:

http://chemistry.anu.edu.au/research/groups/protein-structure-function-and-interactions

SUNDAY 1:00 pm- 1:30pm

Genji Kurisu

Email:

gkurisu@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: OU - Professor (Lab. Protein Crystallography & Protein Databases)

Talk Title: Gallium ferredoxin as a tool to study photosynthetic electron transfer

Abstract: Plant-type ferredoxin (Fd) is an electron transfer protein with a [2Fe-2S] cluster, carrying one-electron from Photosystem I (PSI). To understand the structural basis for the dynamics and efficiency of the electron transfer reaction around Fd, we studied their electron transfer complexes by X-ray crystallography, NMR spectroscopy and flash-absorption spectroscopy. To solve the technical problems, replacement of the paramagnetic iron-sulfur cluster with a diamagnetic gallium-sulfur cluster has been proposed. In order to conclusively determine the chemical composition of the gallium substituted cluster, we solved the crystal structure of GaFd from *Synechocystis* at 1.62 Å resolution and verified its functional complementation using affinity chromatography. Binding of the redox-inactive GaFd to PSI was investigated by flash-absorption spectroscopy, studying both the P700+ decay and the reduction of the native iron Fd in the presence of GaFd. GaFd binding resulted in a slower electron escape from [4Fe-4S] cluster (F_A, F_B) of PSI to exogenous acceptors, in accordance with competitive binding between FdFe and FdGa.

Web:

http://www.protein.osaka-u.ac.jp/crystallography/EngHP

SUNDAY 1:30 pm- 2:00pm

Thomas Huber

Email:

t.huber@anu.edu.au

Institution: **Australian National University,**

Research School of Chemistry.

Position: **Professor of Biological Chemistry**

Talk Title: **3D protein structure determination using lanthanide probes**

Abstract: **Protein 3D structure determination using computational /experimental hybrid methods allows smart information usage by combining molecular modelling with minimal sets of structural data from a range of biochemical and biophysical experiments. Paramagnetic lanthanide ions are particularly attractive probes to generate such data by NMR spectroscopy, because they provide structural restraints which are orientation dependent and long-range (up to 40 Angstrom from the metal centre) due to the strong interaction of the unpaired electron with nuclei in the protein.**

The focus of this talk will be on protein 3D structure determination by assembling super-secondary structure motifs with the help of pseudocontact shift (PCS) restraints for backbone amide protons, where the PCSs are produced from different metal centres. I will show successes and pitfalls of the new assembly algorithm, and discuss how the sparsity of data affects model quality.

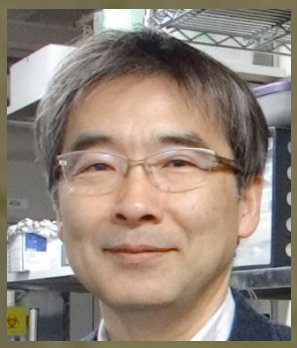
Web:

http://chemistry.anu.edu.au/people/thomas-huber

http://comp-bio.anu.edu.au/

SUNDAY 2:00 pm- 2:30pm

Junichi Takagi



Email:

takagi@protein.osaka-u.ac.jp

Institution: **Laboratory of Protein Synthesis and Expression,**

Institute for Protein Research, Osaka University

Position: **Professor**

Talk Title: **Electron microscopic visualization of LRP6 ectodomain. - N-glycosylation, conformational freedom, and signaling activity -**

Abstract: **LDL-receptor-related protein 6 (LRP6) is a single-pass membrane glycoprotein with a large (~1,300 residues) modular ectodomain, and forms a higher-order signaling platform upon binding Wnt ligands on cell surface. Although multiple crystal structures are available for fragments of the LRP6 ectodomain, we lack a consensus view on the overall molecular architecture of the full-length LRP6 and its dynamic aspects. Here, we used negative-stain electron microscopy (EM) to probe conformational states of the entire ectodomain of LRP6 in solution and found that the four-module ectodomain undergoes large bending motion hinging at the junction between the 2nd and the 3rd modules. Importantly, the extent of inter-domain motion is modulated by evolutionary conserved N-glycan chains present near the joint. Mutations to eliminate specific glycosylation sites impaired basal signaling activity of cell-surface LRP6, suggesting that the glycan-mediated conformational diversification plays important role in the transmembrane signaling, probably by controling the receptor clustering.**

Web: http://www.protein.osaka-u.ac.jp/rcsfp/synthesis/

SUNDAY 2:30 pm- 3:00pm

Malcolm McLeod

Email:

malcolm.mcleod@anu.edu.au

Institution: Australian National University, Research School of Chemistry.

Position: ANU - Level D Academic (Associate Professor)

Talk Title: Of more than PaSing interest – engineering arylsulfatase enzymes for analytical applications

Abstract: The detection and analysis of phase II sulfate metabolites is of growing importance in analytical chemistry. This is in part due to improvements in LCMS technology but also arises due to the important information unveiled by a thorough analysis of phase II metabolism. The analysis of human sulfate metabolites can afford greater retrospectivity for the detection of steroidal agents and provide sensitive markers to distinguish between steroids of exogenous and endogenous origin. Although there are a range of reliable approaches to analyse for phase II metabolites in both humans and animals, the ability to manipulate these metabolites still has limitations. This presentation will detail our work on the enzyme-mediated hydrolysis of steroidal sulfates and engineering of the arylsulfatase from *Pseudomonas aeruginosa*.

Web:

https://researchers.anu.edu.au/researchers/mcleod-md

SUNDAY 3:15pm- 3:45pm

Kiaran Kirk

Email: kiaran.kirk@anu.edu.au

Institution: Australian National University, Research School of Biology

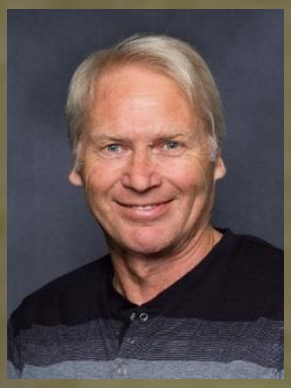
Position: Dean, ANU College of Science

Talk Title: Membrane transport proteins as antimalarial drug targets

Abstract: High-throughput whole-cell phenotypic screens have led to the identification of a raft of potential new antimalarial agents. Using a range of physiological and biochemical assays we have tested the effects of several collections of such compounds on parasite ion homeostasis. The assays have revealed that a significant proportion of the antimalarial agents identified in phenotypic screens against the human malaria parasite, *Plasmodium falciparum*, inhibit membrane transport proteins in the parasite plasma membrane. In particular, the data are consistent with a structurally diverse range of compounds sharing a common mechanism of action, exerting their antimalarial effect via an interaction with the parasite's putative Na^+-efflux ATPase, PfATP4. The parasite's lactic acid efflux transporter, PfFNT, has also emerged as a candidate antimalarial drug target.

Web: http://biology.anu.edu.au/people/kiaran-kirk

SUNDAY 3:45pm- 4:15pm



David Tremethick

Email: david.tremethick@anu.edu.au

Institution: Australian National University,
John Curtin School of Medical Research.

Position: ANU – Head Genome Sciences Department & Group Leader

Talk Title: "What do reproduction and memory have in common? The epigenetic regulator H2A.B"

Abstract: The replacement of histone H2A with its variant forms is critical for regulating all aspects of genome organisation and function. The histone variant H2A.B appeared late in evolution and is most highly expressed in the testis followed by the brain in mammals. This raises the question of what new function(s) H2A.B might impart to chromatin in these important tissues. We have immunopurified the mouse orthologue of H2A.B, H2A.B.3, from testis chromatin and found it to be associated with RNA processing factors and RNA Polymerase (Pol) II. Most interestingly, many of these interactions were inhibited by the presence of endogenous RNA. This histone variant can bind to RNA directly in vitro and in vivo, and associates with transcript RNA at intron-exon boundaries. This suggests that the ability of H2A.B to bind to RNA negatively regulates its capacity to bind to these factors. Unexpectedly, it forms highly decompacted nuclear subdomains of active chromatin that co-localizes with splicing speckles in male germ cells. H2A.B.3 ChIP-Seq experiments revealed a unique chromatin organization at active genes being not only enriched at the transcription start site (TSS), but also at the beginning of the gene body (but being excluded from the +1 nucleosome) compared to the end of the gene. We also uncover a general histone variant replacement process whereby H2A.B.3 replaces H2A.Z at intron-exon boundaries in the testis and the brain, which positively correlates with expression and exon inclusion. Taken together, we propose that a special mechanism of splicing may occur in the testis and brain whereby H2A.B.3 recruits RNA processing factors from splicing speckles to active genes following replacement of H2A.Z.

Web: http://jcsmr.anu.edu.au/groups/groups/tremethick-group

SUNDAY 4:15pm- 4:45pm

John Manners

Email: john.manners@csiro.au

Institution: CSIRO Agriculture and Food

Position: Director

Talk Title: Ag-biotech trends and bringing products to market

Abstract: The global agri-food market is very buoyant with food demand expanding with population growth and increasing wealth in consumers across Asia leading to a desire for healthy, safe and sustainably produced food products. At CSIRO, following these trends, we have brought several novel cereal products to market. These are novel products based on the targeted selection of mutations in specific enzymes. These products include high fibre barley foods which are now available in Japan, and similar high-amylose wheat products as well as gluten-free barley for food and brewing applications. Future mutation targets, including gene editing approaches, will yield nutrient-enhanced and cholesterol-lowering grain products. Constructing pathways through metabolic engineering is more challenging and difficult to commercialise. However, we have a pipeline of novel oil products being delivered by commercial partners and longer term food security options as yield pressure emerges. Now the challenge for CSIRO is to help create an even more dynamic innovation culture in Australia to take agri-food science to market. Several examples of diverse ag-tech innovations that are ripe for commercialisation via agr-food start-ups are emerging and will be described.

Web: http://people.csiro.au/M/J/John-Manners

SUNDAY 5:00pm- 5:30pm

Toshihiko Sugiki

Email:

sugiki@protein.osaka-u.ac.jp

Institution: **Osaka University, Institute for Protein Research.**

Position: **OU - Assistant Professor (Specially Appointed)**

Talk Title: **Molecular Basis of Structure and Function of Lipid Transfer Protein revealed by Solution NMR Spectroscopy**

Abstract: **In cells, lipids play essential roles in vital activities as major components of biomembrane or as lipid-mediators of cellular signal transductions. Following biosynthesis of lipids in the cells, each lipid translocates to organelles and exert their own biological functions on the appropriate organelle membrane. Its intracellular lipid translocation is mainly carried out by lipid transfer proteins (LTPs). Typically, LTPs are multi-domain protein. To exert inter-organelle lipid transfer activity precisely, it is important that each functional domain in the LTPs, such as specific organelle membrane-recognizing domain or lipid binding domain, should demonstrate their individual function. In order to totally coordinate enzymatic activity of LTPs, furthermore, functional activity of each domain must be regulated strictly by proper inter-domain interactions and their functional cross-talking. I will report our structural biological findings elucidating molecular mechanisms of functional regulation of LTPs.**

Web:

http://www.protein.osaka-u.ac.jp/rcsfp/apc/nmr/index

http://www.protein.osaka-u.ac.jp/biophys/bussei

SUNDAY 5:30pm- 6:00pm

Jeremy Tame

Email:

jtame@yokohama-cu.ac.jp

Institution: **Yokohama City University**

Graduate School of Medical Life Science

Position: **Professor**

Talk Title: **MytiLec - a novel beta-trefoil lectin**

Abstract: **Recently a novel lectin was discovered in shellfish, and found to have unusual ligand specificity that allowed it selectively to enter and kill certain types of cancer cell. The crystal structure shows the protein to have the well-known beta-trefoil fold, but with a novel sequence unrelated to previously studied proteins. An artificial form of the protein has been engineered as a first step towards creating clinically useful molecules for cancer detection and treatment.**

Web:

http://www.tsurumi.yokohama-cu.ac.jp/pdl/PDL/Jeremy.html

SUNDAY 7:20pm- 7:30pm

Toru Fujiwara

Email: fujiwara@ist.osaka-u.ac.jp

Institution: Osaka University,

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Position: Associate Executive Director, Global Engagement office

Professor, Associate Dean, Graduate School of Information Science and Technology

It is our great pleasure and honor to welcome you to Osaka University for the Second IPR/RSC Joint Symposium.

We recognize collaborative works between the IPR (Institute for Protein Research) at Osaka University and RSC (Research School of Chemistry) at the Australian National University including the successful First Joint Symposium held in Australia in November 2015. Therefore, we believe the discussions on protein structure and function as well as related subjects in this symposium are fruitful and will yield further collaborative research, which will build stronger relations between both Universities.

Finally, we would like to thank you all for your participation. We hope all of you find the symposium stimulating and have an enjoyable stay in Osaka.

SUNDAY 7:30pm- 8:30pm

Kyosuke Nagata

Email: nagata.kyosuke.fm@un.tsukuba.ac.jp

Institution: University of Tsukuba

Position: President

Talk Title: The Nature of Japan's Changing University Scene

Abstract: As with the society where we live, the university is just in turbulent times. In this globalized society, there are a number of issues to be solved such as population and food problems, economic competition and disparity, challenges related to energy and pollution, environmental problems, emerging/re-emerging infectious diseases, and so on. It is obvious that development of science and technology and human resource driving the future is essential to overcome these. To this end, it is highly expected that the university plays important roles, and thereby should be reformed. In this talk, I would like to introduce how Japanese universities, in particular national universities are changing based on recent Japanese government policy for higher education. In addition, some cases of excellent trials by universities will be presented for discussion with audience.

Web:

http://www.tsukuba.ac.jp

http://www.tsukuba.ac.jp/president/

MONDAY 8:30am- 9:00am

Johannes Buchner

Email:

johannes.buchner@tum.de

Institution: Department of Chemistry,

Technical University of Munich, Germany

Position: Professor

Talk Title: Molecular chaperones – cellular machines for protein folding

Abstract: Cells have developed a quality control system that ensures that the proteome folds correctly, keeps its native conformation and that unproductive side reactions are prevented. The key elements of this defence system are molecular chaperones. These machines of protein folding share the remarkable ability of specifically recognizing non-native proteins and assisting their folding to the native state. With a view to define the key traits of different chaperone machines, we set out to reconstitute their mode of action using purified components. Our analysis reveals sophisticated regulatory and control elements to adjust chaperone activity.

Web: https://www.biotech.ch.tum.de/index.php?id=555&L=0

MONDAY 9:00am- 9:30am

Damien Hall

Email:

damien.hall@anu.edu.au

damien.hall@protein.osaka-u.ac.jp

Institution: **Australian National University, Research School of Chemistry.**

Osaka University, Institute for Protein Research.

Position: **ANU - Level C Academic (Senior Research Fellow)**

OU - Associate Professor (Specially Appointed)

Talk Title: **Folding and Unfolding - Research as a Cross-Appointed Fellow**

Abstract: **A summary is given about three years of research on protein structure and function performed under the Cross-Appointment Fellowship Scheme existing between the Institute for Protein Research (Osaka University) and the Research School of Chemistry (Australian National University). The major focus of the talk is research relating to the measurement and simulation of protein folding/unfolding and amyloid fibre growth. This research is described in light of current day knowledge of how amyloid relates to disease.**

Web:

http://chemistry.anu.edu.au/research/groups/physical-biochemistry-disease

http://www.protein.osaka-u.ac.jp/en/laboratories/multiscale-structural-biology

MONDAY 9:30am- 10:00am

Hironobu Hojo

Email:

hojo@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: Professor

Talk Title: Protein science based on chemical synthesis

Abstract: We have been developing a facile method for protein synthesis, which can be applicable to prepare simple proteins as well as post-translationally modified, site-specifically labeled proteins and so on. The basic strategy is to synthesize protein segments by the solid-phase method and condense them chemoselectively to assemble the entire protein. In this presentation, I will talk about recent progress of the method. The one is to cope with the low solubility problem during the synthesis. When we divide the target proteins to several segments, some of them are quite insoluble to common solvents used for the purification and ligation to make the total synthesis impossible. Using glycosylated interleukin-2 as a model, we developed a novel method to solve this problem.

The other is to improve the entire synthetic process. In the previous syntheses, the purification by HPLC is required after each ligation reaction, which decreases the total yield of the product. By combining the segments with different reactivity, we recently developed the one-pot four-segment ligation, in which four peptide segments can be condensed without purification till the end of the ligation reactions. The detail of the method will be shown using human superoxide dismutase-1 as a model.

Web: http://www.protein.osaka-u.ac.jp/organic/english.html

MONDAY 10:00am- 10:30am

Lara Malins

Email:

u1050766@anu.edu.au

malins@scripps.edu

Institution: **Australian National University, Research School of Chemistry.**

The Scripps Research Institute, La Jolla, California.

Position: **ANU - Level B Academic (Research Fellow) – beginning Dec. 2017**

TSRI - Postdoctoral Fellow, Prof. Phil Baran

Talk Title: **Late-Stage Peptide Modifications: A Growing Toolbox**

Abstract: **Synthetic strategies for the targeted functionalization of unprotected peptides are crucial to the development of new residue-specific bioconjugation and protein modification reactions. This talk will summarize three recent additions to the peptide modification toolbox: 1) a thermodynamic peptide macrocyclization strategy; 2) strain-release cysteine functionalization; and 3) a cross-coupling approach to unnatural amino acids. The potential to extend these enabling methods to residue-specific protein modifications will be discussed.**

Web: https://www.linkedin.com/in/lara-malins-a918554/

MONDAY 10:45am- 11:15am

Mamoru Takizawa

Email:

takizawa@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: Ph.D. student in third year

Talk Title: The Glu residue of laminin γ chain comprises a bipartite integrin recognition site together with LG1–3 domains of laminin α chain

Abstract: Laminin is a basement membrane protein composed of α, β, and γ chains. Laminin elicits a variety of cellular responses through interactions with cell surface receptors, particularly integrin. Accumulating evidence indicated that the integrin-binding site is mapped to the three LG domains of α chain (LG1–3), whose integrin-binding activity is strictly dependent on the C-terminal 9 residues of γ chain (γ-tail), particularly the Glu residue at the third position from the C-terminus. However, it remains to be elucidated whether the Glu residue in the γ-tail contributes to adopting an active LG1–3 conformation for integrin recognition or directly interact with integrins. Here, I sought to determine the role of the γ-tail in the laminin-integrin interaction by X-ray crystallography combined with a series of biochemical analyses. Based on the results of these experiments, I will discuss the molecular mechanism by which integrin recognizes laminin.

Web: http://www.protein.osaka-u.ac.jp/matrixome/

MONDAY 11:15am- 11:45am

Marco Cassarotto

Email: Marco.Casarotto@anu.edu.au

Institution: Australian National University, John Curtin School of Medical Research.

Position: ANU - Level D Academic (Associate Professor)

Talk Title: Key molecular interactions in skeletal EC coupling machinery

Abstract: Recent advances in Cryo-EM has meant that we now have access to high-resolution structures for both skeletal muscle proteins CaV1.1 and RyR1. However, the exact nature of how they communicate with each other is the next challenge that must be overcome to fully understand the mechanisms that underlie excitation contraction (EC) coupling. It is clear both the α1s and β1a subunits of CaV1.1 are key players in this interactive system and mutations within these subunits have been identified as being responsible for a range of skeletal muscle-associated diseases. In this study, we aim to define the structural and interactive framework involving key regions of the skeletal muscle machinery. We have recently determined the structure of CaV1.1 β1a using X-ray. The b1a subunit was found to interact strongly with a α1s I-II loop peptide, AID (Kd ~4 nM) and moderately with the α1s II-III loop through an SH3 domain (~3 μM). It was noted that in the presence of the AID peptide, no binding of the II-III loop to β1a was detected. This is a significant observation indicating a degree of crosstalk between the I-II and II-III loop interaction sites. We propose that depolarisation of the transverse t-tubule leads to perturbation of I-II loop binding to the β1a subunit leading to other interactive downstream effects including binding of the II-III loop. A more recent discovery has been the essential role that the accessory protein STAC3 plays in the EC coupling process. It has been proposed that this protein acts the bridge between the proteins CaV1.1 and RyR1 proteins. Here we evaluate the ability of STAC3 to activate RyR1 using single channel measurements and endeavour to map the binding site of STAC3 on RyR1.

Web: http://jcsmr.anu.edu.au/groups/groups/casarotto-group

MONDAY 11:45am- 12:15pm

Nobuaki Okumura

Email: nokumura@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: Associate Professor

Talk Title: Enzymatic mechanisms of dipeptide breakdown

Abstract: Dipeptides are yielded in metabolic processes such as dietary protein digestion, protein re-uptake in the kidney and intracellular protein turnover. There are also dipeptides that are synthesized from component amino acids by specific enzyme reactions. The latter include carnosine (β-ala-His), which is stored at high concentrations in the muscles and the brain, and may be implicated in anti-oxidation, pH buffering, and neuronal modulation. Tissues express various dipeptidases, each of which have specific tissue distribution and specific spectrum of substrate specificity. Carnosine dipeptidase 2 (CN2), is a mammalian cytosolic metallopeptidase highly expressed in the small intestine, kidney and specific regions in the brain. CN2 had been thought to be a Mn^{2+}-dependent enzyme, but our recent analysis using native mass spectrometry shows that Zn^{2+} binds to CN2 with a higher affinity than Mn^{2+}. We also found that the Zn^{2+} form of CN2 has an enzymatic activity, while its substrate specificity is different from that of the Mn^{2+} form. These and further studies demonstrate the essential roles of CN2 in intracellular dipeptide hydrolysis in mammals.

Web: http://www.protein.osaka-u.ac.jp/laboratories/metabolism

MONDAY 1:30pm- 2:00pm

Richard Callaghan

Email: richard.callaghan@anu.edu.au

Institution: Research School of Biology and Medical School, The Australian National University,

Position: ANU - Level D (Associate Professor)

Talk Title: How does P-glycoprotein bind so many drugs?

Abstract: P-glycoprotein (P-gp) gained notoriety for its role in conferring drug resistance to an astonishing number of cytotoxic drugs used in oncology. The protein is able to confer resistance by preventing sufficient accumulation of chemotherapy drugs within cancer cells. P-gp is one of three multidrug efflux pumps in humans and their actions have been the focus of considerable research. Recently, an x-ray crystallography based structure has been presented for P-gp and has been touted as the "missing piece in the puzzle" to generate a mechanistic understanding of this protein. Has this been achieved yet and is there any benefit to further biochemical studies on P-gp? Our continuing research focus is to provide a dynamic understanding of the drug translocation process of P-gp. In particular, we aim to locate the drug binding site(s) on the protein and describe their communication with the energy providing domains. This information will be used to describe the precise steps involved in multidrug transport at a molecular level.

Web:

http://biology.anu.edu.au/research/labs/callaghan-lab-human-disease-and-membrane-transport

MONDAY 2:00pm- 2:30pm

Joji Mima

Email:

Joji.Mima@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: OU - Associate Professor

Talk Title: Dissecting the specificity of Rab-mediated membrane tethering in a chemically defined reconstitution system

Abstract: Membrane tethering is the most critical processes to determine the specificity of membrane trafficking in eukaryotic cells, delivering the correct sets of cargoes (proteins etc.) to the correct locations (organelles, the extracellular space etc.). Among miscellaneous key protein components in membrane trafficking (SNAREs, SNARE chaperones, Rab-family GTPases, and Rab effectors etc.), Rab proteins and specific sets of Rab effectors have been reported to be responsible for membrane tethering. Nevertheless, whether and how indeed Rabs and Rab effectors work together to drive membrane tethering still remains enigmatic. Here, we reconstituted membrane tethering reactions in a chemically defined system from synthetic liposomal membranes and purified human Rab proteins. Our reconstitution studies now support the novel concept that Rabs provide a *bona fide* membrane tether to physically link two distinct lipid bilayers, and Rab effectors can regulate the Rab-mediated membrane tethering reactions (Tamura & Mima, *Biol Open*, 2014; Inoshita & Mima, *J Biol Chem*, 2017).

Web: http://www.protein.osaka-u.ac.jp/en/laboratories/mima-en

MONDAY 2:30pm- 3:00pm

Jen Taylor

Email:

jen.taylor@csiro.au

Institution: CSIRO Agriculture and Food

Position: Research Group Leader, Genome Science for Crop Performance

Talk Title: Opportunities for proteomics in emerging agricultural crop genomes.

Abstract: The rapid emergence of deeply characterised genomes in important agricultural crops presents opportunities to enhance and expand understanding of biological function, as is manifested through protein function and interactions. Within cereal species, the recent release of complex reference genomes, such as wheat and large pan-genomic resources, such as those in rice, together present unprecedented opportunities to use i) comparative genome analysis strategies; ii) evolutionary models and iii) data integration to bring together the strengths of proteomics and genomics. This talk will present examples of research that utilises these opportunities and will focus on the implications protein:DNA and protein:protein interactions to create important regulatory networks critical to plant function and performance.

Web: http://people.csiro.au/T/J/Jen-Taylor

MONDAY 3:00pm- 3:30pm

Hafna Ahmed

Email:

hafna.ahmed@anu.edu.au

Institution: **Australian National University, Research School of Chemistry**

Position: **ANU - Level A Academic (Postdoctoral Fellow)**

Talk Title: **Cofactor F_{420}: uncovering new roles in mycobacterial pathogens**

Abstract: **The rare cofactor F_{420} is important in mycobacterial pathogens like *Mycobacterium tuberculosis* to survival oxidative stress and to recover from dormancy. However, the F_{420}-dependent mechanisms involved in tese processes remain largely unknown. We present the functional characterisation of the largest mycobacterial F_{420} utilizing protein family called the flavin/deazaflavin dependent oxidoreductases (FDORs). Their cofactor preferences, sequence similarity and existing characterizations allowed classification into new functional groups. This includes the $F_{420}H_2$-dependent quinone reductases that can promiscuously activate 4-nitroimidazole pro-drugs approved against multi-drug resistant *M. tuberculosis*. $F_{420}H_2$-dependent fatty acid saturases and $F_{420}H_2$-dependent biliverdin reductases (F-BVRs) were also identified, where the F-BVR Rv2074 from *M. tuberculosis* reduces biliverdin-IXα to bilirubin-IXα, a potent antioxidant. Lastly, the widespread use of F_{420} in the broader bacterial community is demonstrated, alluding to the undiscovered roles of F_{420} in bacterial metabolism.**

Web: https://researchers.anu.edu.au/researchers/ahmed-fh

MONDAY 3:45pm- 4:15pm

Junichi Higo

Email:

higo@protein.osaka-u.ac.jp

Institution: Institute for Protein Research, Osaka University.

Position: Guest Professor

Talk Title: Computational study for protein-protein interactions based on the first-principle approach

Abstract: Investigation of protein-protein or protein-ligand interactions at an atomic resolution is crucially important for understanding protein functions. If a computational procedure can reproduce the protein-protein interactions and their complex form, the technique is useful not only for fundamental research area but also for drag-design. I have been developing the computational approach (computer simulation techniques) for exploring the protein conformational variety. The protein molecules are treated realistically: i.e., flexible and solved explicitly in solvent. The protein molecules move according to equation of motion. I will introduce results from my computation.

Web: http://www.protein.osaka-u.ac.jp/rcsfp/pi/members_en.html

MONDAY 4:15pm- 4:45pm

Karmen Condic-Jurkic

Email:

karmen.condic-jurkic@anu.edu.au

Institution: Australian National University, Research School of Chemistry.

Position: ANU - Level A Academic (Postdoctoral fellow)

Talk Title: MDbox – a cloud-based repository and analysis toolkit for molecular dynamics simulations

Abstract: Computational techniques such as molecular dynamics (MD) simulations are increasingly used to study the interactions of biomolecules and/or materials at an atomistic level. MD simulations are still computationally costly, requiring supercomputer access and significant scientific input. MDbox represents a prototype for an open access repository for MD simulation datasets. MDbox aims to provide a platform for storing and sharing trajectories and their corresponding input files, which should improve documentation of commonly used protocols and enhance the replicability and reproducibility of simulations. Ultimately, MDbox should make collaboration and data exchange easier and provide an alternative for making research publicly available and citable.

In our information-driven era, this open data approach is of tremendous value for further development of computational modelling and for cross-disciplinary researchers in both academia and industry. The ability to access a large number of simulations in a single repository will create unprecedented opportunities for research into "big data" analysis and mining techniques.

Web: http://www.mdbox.org/

MONDAY 4:45pm- 5:15pm

Kazunari Iwamoto

Email:

kiwamoto@protein.osaka-u.ac.jp

Institution: Laboratory of Cell Systems, Institute for Protein Research, Osaka University.

Position: Assistant Professor

Talk Title: Formation of NF-kappaB super enhancer regulated by chromatin structural changes

Abstract: Super enhancer which is large cluster of transcriptional enhancers has been proposed as one of the transcriptional regulation mechanisms that control cell type specific gene expressions. Recent study showed that nuclear factor kappa B (NF-κB), which plays an essential role in B cell maturation, functions as super enhancer. However, it has been still unclear how NF-κB super-enhancer is regulated in B cell.

In this talk, we focus on the relationship between super-enhancer formation, NF-κB enrichment and chromatin structure. Our analysis results using various sequence data demonstrate that chromatin structural changes at NF-κB binding motif control super enhancer formation and the associated gene expression.

Web:

http://www.protein.osaka-u.ac.jp/cell_systems/

https://scholar.google.co.jp/citations?user=IxIb06MAAAAJ&hl=ja

MONDAY 5:15pm- 5:45pm

Steve Swain

Email: steve.swain@csiro.au

Institution: CSIRO Agriculture and Food

Position: Research Director

Breakthrough Genetic Technologies

Talk title: Genetic regulation of wheat spike development

Abstract:

A major target for genetic improvement of cereals, including wheat, is to increase the number of fertile florets/grains per plant. One way to achieve a potential increase in grain number per spike is to alter spike (inflorescence) architecture, by modifying the number of fertile florets produced by each spikelet, the number of spikelets at each node, or the number of spikelets per spike. We are using genetic mapping and induced mutants to investigate the control of spike architecture and yield potential in wheat. Our results suggest that the major flowering genes regulate spike architecture and have direct effects on yield potential beyond controlling heading date.

Using forward genetic screens, we have also identified new alleles of the major domestication gene, *Q*. The advantages of free threshing in wheat led to the selection of the *Q* allele, which is now present in almost all modern wheat varieties. *Q* and the pre-domestication allele, *q*, encode an AP2 transcription factor, with the domesticated allele conferring a free-threshing character and a subcompact (i.e. partially compact) inflorescence (spike). We demonstrate that mutations in the miR172 binding site of the *Q* gene are sufficient to increase transcript levels via a reduction in miRNA-dependent degradation, consistent with the conclusion that a single nucleotide polymorphism in the miRNA binding site of *Q* relative to *q* was essential in defining the modern *Q* allele. We describe novel gain- and loss-of-function alleles of *Q* and use these to define new roles for this gene in spike development. *Q* is required for the suppression of 'sham ramification', and increased *Q* expression can lead to the formation of ectopic florets and spikelets (specialized inflorescence branches that bear florets and grains), resulting in a deviation from the canonical spike and spikelet structures of domesticated wheat.

Web: https://www.csiro.au/en/Research/AF

http://people.csiro.au/S/S/Steve-Swain

MONDAY 7:30pm- 8:30pm

Yuji Goto

Email:

gtyj8126@protein.osaka-u.ac.jp

Institution: **Osaka University, Institute for Protein Research.**

Position: **Professor**

Talk Title: **The Interesting Life Story of Yukichi Fukuzawa**

Web:

http://www.protein.osaka-u.ac.jp/en/laboratories/yoeki-en

http://www.protein.osaka-u.ac.jp/physical/index.html

TUESDAY 8:30am- 9:00am

Vittorio Bellotti

Email:

v.bellotti@ucl.ac.uk

Institution: **University College London, London (UK), Centre for Amyloidosis and Acute Phase Proteins**

Position: **Professor of Medical Biochemistry Metabolism & Experimental Therapeutics**

Talk Title: **Proteolysis and transthyretin amyloidogenesis: a new way of reading an old story**

Abstract: **The chemical characterization of *ex-vivo* amyloid fibrils in systemic amyloidosis suggests that most of the constitutive culprit proteins are cleaved. The role of selective proteolytic cleavage on the fibrillogenesis of globular protein has been debated for decades but yet mysterious. The paradigmatic example of transthyretin (TTR) amyloidosis illuminates on the slow and continuous progress made in the last 20 years towards a better understanding of the link between the structural dynamics of amyloidogenic proteins and their special susceptibility to proteolytic cleavage. A region of local instability is well tolerated in the TTR assembled homotetramer, but a selective proteolytic cleavage drastically affects its stability. The TTR model reveals how local unfolding and proteolytic cleavage may represent two obligate partners equally responsible for the early pathogenic event of the amyloid cascade.**

Web: http://ucl.ac.uk/amyloidosis

TUESDAY 9:00am- 9:30am

Hideki Mochizuki

Email: hmochizuki@neurol.med.osaka-u.ac.jp

Institution: Department of Neurology,
Osaka University Graduate School of Medicine

Position: Professor and Chairman

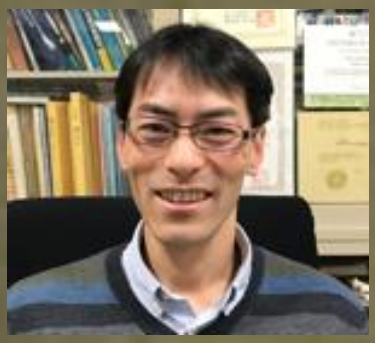
Talk Title: Structure and Function of α synuclein

Abstract: Lewy bodies (LBs), which mainly consist of α-synuclein (α-syn), are neuropathological hallmarks of patients with Parkinson's disease (PD). The fine structure of LBs is unknown, and LBs cannot be made artificially. Thus, we used synchrotron Fourier transform infrared micro-spectroscopy (FTIRM) to analyse the fine structure of LBs in the brain of PD patients at Spring 8. In addition, we attained the detection sensitivity enhancement and the measurement time savings by ultrasonication and has already developed a device for performing these measurements automatically. A combined system "HANABI (HANdai Amyloid Burst Inducer)" for inducing and detecting amyloid fibrils automatically was made by Prof. Goto and his group. HANABI will be useful for a high-throughput assay of the amyloidogenicity of proteins. We have already had interesting results using diseased samples measured by HANABI.

Web:

http://www.med.osaka-u.ac.jp/eng/introduction/research/integrated/neurology

TUESDAY 9:30am- 10:00am



Hirotsugu Ogi

Email:

ogi@prec.eng.osaka-u.ac.jp

Institution: Osaka University, Graduate School of Engineering.

Position: Professor

Talk Title: Ultrasonic cavitation and fibrillation phenomenon of protein

Abstract: Since the discovery of ultrasonically accelerated protein-fibrillation phenomenon [1], ultrasonic irradiation has been recognized as a promising methodology for studying proteins' aggregation reactions. The detailed mechanism on the promotion of aggregation, however, remains unclear. We have studied systematically aggregation reactions of Aβ peptide and insulin with various acoustic pressures, frequencies, and duty cycles using our originally developed instrument, and found some important characteristics of cavitation for making fibrillation possible [2-4].

[1] Y. Ohhashi, Y. Kihara, H. Naiki, and Y. Goto, J. Biol. Chem. 280, 32843-32848 (2005).

[2] K. Nakajima, H. Ogi, K. Adachi, K. Noi, M. Hirao, H. Yagi, and Y. Goto, Sci. Rep. 6, 22015 (2016).

[3] K. Nakajima, D. Nishioka, M. Hirao, M. So, Y. Goto, and H. Ogi, Ultrason. Sonochem. 36, 206-211 (2017).

[4] K. Nakajima, M. So, K. Takahashi,Y. Tagawa, M. H, Y. Goto, and H. Ogi, J. Phys. Chem. B 121(12), 2603-2613 (2017).

Web:

http://www-qm.prec.eng.osaka-u.ac.jp/

TUESDAY 10:00am- 10:30am

Yuji Goto

Email:

gtyj8126@protein.osaka-u.ac.jp

Institution: Osaka University, Institute for Protein Research.

Position: Professor

Talk Title: Revisiting supersaturation as a factor determining amyloid fibrillation

Abstract: Amyloid fibrils involved in various diseases are formed by a nucleation-growth mechanism, similar to the crystallization of solutes from solution. Solubility and supersaturation are two of the most important factors determining crystallization of solutes. Moreover, crystallization competes with glass formation in which solutes collapse into amorphous aggregates. Recent studies on the formation of amyloid fibrils and amorphous aggregates indicate that the partition between distinct types of aggregates can be rationally explained by a kinetic and thermodynamic competition between them. Understanding the role of supersaturation in determining aggregation-based phase transitions of denatured proteins provides an important complementary point of view to structural studies of protein aggregates.

Reference: So et. al. (2016) Curr. Opin. Struct. Biol. 36:32-39.

Web:

http://www.protein.osaka-u.ac.jp/en/laboratories/yoeki-en

http://www.protein.osaka-u.ac.jp/physical/index.html

TUESDAY 10:45am- 11:15am

Chris Easton

Email:

chris.easton@anu.edu.au

Institution: **Australian National University, Research School of Chemistry.**

Position: **Level E Academic (Professor)**

Talk Title: **A Radical Approach to Enzyme Biotechnology**

Abstract: **Fundamental studies of free radical reactions of peptides and proteins will be discussed in the context of regulation of hormone production in human cancers. This will lead in to enzyme biotechnology for sustainable agriculture and manufacturing where work within the CSIRO Energy Transformed Flagship Cluster on Biofuels, developing enzyme biotechnology for the conversion of biomass to liquid transport fuels, and in collaboration with the Grains Research and Development Corporation, towards enzyme-catalysed production of crop nutrients, will be discussed.**

Web:

http://chemistry.anu.edu.au/research/groups/biochemical-reactions-molecular-recognition

TUESDAY 11:15am- 11:45am

Tom Macpherson

Email:

tom@tk.med.kyoto-u.ac.jp

Institution: **Kyoto University, Graduate School of Medicine.**

Osaka University, Institute for Protein Research.

Position: **KU – Postdoc Researcher**

OU – Assistant Professor

Talk Title: **Dopamine D2L receptors control behavioral flexibility**

Abstract: **Altered functioning of the Nucleus Accumbens (NAc) is known to contribute to the etiology of several neuropathologies associated with impaired behavioural control, including schizophrenia and drug addiction. Neurons within the NAc can be divided into two distinct classes, dopamine D1- or D2-receptor expressing medium spiny neurons (D1-/D2-MSNs). We used a combination of molecular and behavioural techniques to examine the role of NAc D1- and D2-MSNs in the acquisition and reversal learning of a place discrimination task. Blockade of activity in NAc D1- and D2-MSNs did not alter acquisition of the task, however, suppression of activity in D2-MSNs impaired reversal learning and increased perseverative errors. Additionally, global knockout of the dopamine D2L receptor isoform produced a similar behavioral phenotype to D2-MSN-blocked mice. These results suggest that D2L receptors and NAc D2-MSNs act to suppress the influence of previously correct behavioral strategies allowing transfer of behavioral control to new strategies, and indicate that D2L receptors and NAc D2-MSNs may provide efficacious therapeutic targets for treating neuropathologies associated with loss of behavioral control.**

TUESDAY 11:45am- 12:15pm

Christoph Nitsche

Email:

christoph.nitsche@anu.edu.au

Institution: The Australian National University, Research School of Chemistry

Position: Feodor Lynen Research Fellow (Alexander von Humboldt Foundation)

Talk Title: Covalent-Reversible Protein Modification – Opportunities from the Main Group Chemistry Toolbox

Abstract: Small compounds that covalently bind to larger biomolecules are uniquely useful for multiple purposes, including drug target validation and to probe function, cellular localisation and dynamics of the target molecule. In contrast to commonly employed irreversible modifiers, my work focuses on previously neglected covalent *reversible* probes and inhibitors, as they allow greater selectivity.

Several underexplored main group elements offer unique binding characteristics for this purpose. Combined with organic reporter molecules they can enable site-selective and reversible bioconjugation.

The presentation will focus on boron-based probes and inhibitors to study enzymes of emerging viral pathogens as well as novel strategies to self-assemble probe and biomolecule mediated by arsenic, antimony or bismuth.

Web: http://chemistry.anu.edu.au/people/christoph-nitsche

TUESDAY 12:15pm- 12:45pm

Kohei Takeshita

Email:

takeshita@protein.osaka-u.ac.jp

Institution: **Laboratory of Supramolecular Crystallography**

Osaka University, Institute for Protein Research.

Position: **OU - Assistant Professor (Specially Appointed)**

Talk Title: **Structural & Functional Studies on Voltage-Gated Proton Channel.**

Abstract: **Voltage-gated proton channel, which was recently identified in 2006[1], consists of a membrane voltage sensor that is found in canonical voltage-gated ion channels such as Kv or Nav and cytoplasmic coiled-coil. VSOP was widely found in human from plant plankton. The most popular function of VSOP is production of superoxide in phagocytes coupled with NADPH oxidase to eliminate pathogens. Also, VSOP has been suggested to regulate motility through activating pH-sensitive calcium channels in human sperms. Moreover, VSOP regulates pH environment coupled Na^+/H^+ exchanger in cardiac muscle cells. Interestingly, VSOP has the proton permeation pathway in intermolecular of voltage-sensor domain, however canonical voltage-sensor domains do not permeate ions. In my presentation, I would like to talk about the crystal structure of VSOP[2,3] focused proton permeation or voltage sensor motion depending on membrane voltage changes.**

1. M. Sasaki, Y Okamura *et al*. Science 312 (2006) .
2. Y Fujiwara, T Kurokawa, K Takeshita *et al*. Nat. comm. 816 (2012). .
3. K. Takeshita *et al*. Nat. Strcut. Mol. Biol. 21 (2014) .

Web: http://www.protein.osaka-u.ac.jp/rcsfp/supracryst/

Guest Poster Presenters: Abstracts and Biographies

Mr. Hendrik MAAT: Variability in Amyloid Kinetics

Abstract: We have developed experimental and computational techniques for performing and analysing 96 well pate assays using hen egg white lysozyme as the model aggregating system. Developed data reduction techniques for decomposing curves into four characteristic parameters with analysis of variance for each parameter set are presented. Systematic method for analysis of an experimenter's level of skill is examined using an asymptotic plot of mean and variance for independent measurement sets.

Email: hendrik.maat@anu.edu.au **Address: Australian National University, Research School of Chemistry.**
Position: (i) ANU - Level 7 Professional Staff (Senior Technical Officer) (ii) Part time PhD student

Mr. Thomas LOAN: Lysates for Multi-Enzymatic Synthesis

Abstract: Nucleotide triphosphates (NTPs) are widely used in modern biochemical research and therefore are attractive synthetic targets. Although enzymatic synthesis allows highly specific and efficient catalysis, it typically requires expensive co-factors such as ATP. To overcome this we utilized ATP recycling with endogenous acetate kinase present in cell lysate and cheap to prepare acetyl phosphate. These cheap alternative protocols showcase the potential of free lysate based ATP recycling with acetyl phosphate.

Email: Thomas.Loan@anu.edu.au **Address: Australian National University, Research School of Chemistry.**
Position: ANU – Ph.D. Student

Mr. Ryota WAKAYAMA: Aggregate Turbidity in AUC Experiments

Abstract: Amyloid fibrils are ordered aggregates of peptides or proteins that contribute to many diseases. A number of studies have measured amyloid size distributions by sedimentation velocity (S.V.) experiments performed in a spectrophotometer equipped analytical ultracentrifuge (AUC) typically recording at 280 nm. Due to the large size of the aggregates, it is possible that a large fraction of measured distribution is actually due to signal derived from light scattering rather than protein absorbance.

Email: ryota.wakayama@bio.eng.osaka-u.ac.jp ; u1031653@anu.edu.au **Address: Australian National University Research School of Chemistry and John Curtin School of Medical Research. Osaka University, Faculty of Engineering Science.**
Position: Masters Course Student (Osaka) and Occupational Trainee (Australia)

Mr. Spencer RICHARDSON: Ryanodine Receptor Structure/Function

Abstract: Not supplied at time of printing.

Email: spencer.richardson@anu.edu.au **Address: Australian National University, John Curtin School of Medical Research**
Position: PhD Student

Ms. Elmira BAHRAMINEJAD: Amyloid Aggregation from Milk Proteins

Abstract: Amyloid deposits are found in bovine mammary tissue within calcified proteinaceous deposits, known as corpora amylacea, wherein the presence of several milk proteins have been reported. Caseins form the major fraction of milk proteins and hence are studied for understanding the proteopathic mechanisms underlying amyloidogenesis. In the current study, we aimed to investigate the amyloid fibril forming propensity of αS1- and β-casein which have not yet been reported.

Email: elmira.bahraminejad@anu.edu.au **Address: Australian National University Research School of Chemistry**
Position: PhD Student (Osaka)

Dr. Guglielmo VERONA: Nanobodies Prevents Amyloidogenesis

Abstract: Amyloid conversion of β2-microglobulin (β2m) has been extensively investigated. Inhibitors of wild type β2m, such as doxycycline and analogues and a specific nanobody, Nb24, have been previously investigated using non-physiological conditions for protein aggregation. Here we focus our studies on the inhibition of the amyloidogenic natural D76N variant,that is associated with hereditary familial amyloidosis and forms fibrils in physiologically relevant conditions.

Email: g.verona@ucl.ac.uk **Address: University College London – Centre for Amyloidosis and Acute Phase Proteins.**
Position: Research Associate

Mr. Shouvik ADATYA: STAC3 in Muscle Contraction

Abstract: STAC3 is a recently discovered protein associated with excitation contraction (EC) coupling in skeletal muscle. It consists of 360 amino acid residues and contains two SH3 protein-interaction domains and a glutamic acid rich domain. In humans, a mutation in STAC3 is implicated in Native American Myopathy (NAM), a disease that causes congenital weakness, cleft palate and a predisposition to malignant hyperthermia.

Email: shouvik.aditya@anu.edu.au **Address: Australian National University, John Curtin School of Medical Research.**
Position: PhD Student

Mr. Zuben BROWN: Novel labelling for electron microscopy

Abstract: Unambiguously identifying domains of macromolecular complexes using electron microscopy (EM) can be difficult if only intermediate resolutions are obtained. In these cases antibody labelling can provide localization information by comparisons with unbound control structures, however, this relies on the availability of a panel of high affinity antibodies for each site of interest. I will present a novel EM labelling method that exploits interactions between small peptide and a single high affinity antibody allowing for identification of various domains throughout a protein without the need to generate a range of antibodies.

Email: zuben@protein.osaka-u.ac.jp **Address: Osaka University, Institute for Protein Research.**
Position: DSc Student

Poster Presentations 1st Floor Tea Room (Lunch Hours / Breaks)

- Poster set up from 9am Sunday 3rd – 5th of December

Name	Poster Presentation Title
1. Mr. Hendrik MAAT	Variability in Amyloid Kinetics (ANU)
2. Mr. Thomas LOAN	Lysates for Multi-Enzymatic Synthesis (ANU)
3. Mr. Ryota WAKAYAMA	Aggregate Turbidity in AUC Experiments (ANU)
4. Mr. Spencer RICHARDSON	Ryanodine Receptor Structure / Function (ANU)
5. Ms. Elmira BAHRAMINEJAD	Amyloid Aggregation from Milk Proteins (ANU)
6. Dr. Guglielmo VERONA	Nanobodies Prevents Amyloidogenesis (UCL., UK)
7. Mr. Shouvik Adatya	STAC3 in Muscle Contraction (ANU)
8. Mr. Zuben Brown (PI Junichi TAKAGI)	Novel protein labelling technologies for EM (IPR)
9. PI Hironobu HOJO	Laboratory of Protein Organic Chemistry
10. PI Mariko OKADA	Laboratory of Cell Systems
11. PI Yoshie HARADA	Laboratory of Nanobiology
12. PI Yuji GOTO	Laboratory of Protein Folding
13. PI Toshimichi FUJIWARA	Laboratory of Molecular Biophysics
14. PI Genji KURISU	Laboratory of Protein Crystallography
15. PI Akira SHINOHARA	Laboratory of Genome/Chromosome Functions
16. PI Takahisa FURUKAWA	Laboratory of Molecular/Developmental Biology
17. PI Takatoshi HIKIDA	Laboratory for Advanced Brain Functions
18. PI Toshifumi TAKAO	Laboratory of Protein Profiling/Functional Proteomics
19. PI Atsushi NAKAGAWA	Laboratory of Supramolecular Crystallography
20. PI Haruki NAKAMURA	Laboratory of Protein Informatics
21. IAP Junko KANOH	Laboratory of Nuclear Network
22. IAP Joji MIMA	Laboratory of Membrane Protein Chemistry