# 23<sup>rd</sup> IUPAC Conference on Physical Organic Chemistry

# ICPOC23



# SYDNEY AUSTRALIA

## **Conference Programme**

### Welcome

It is with great pleasure that we welcome you to the University of New South Wales, Sydney and to the 23<sup>rd</sup> IUPAC Conference on Physical Organic Chemistry (ICPOC23). The ICPOC series of biennial conferences stretches back to the first meeting in 1972 in Switzerland. Since then, meetings have been held all over the world – but this is the first time that it has been held in Australia!

With its roots in relating molecular structure to chemical behaviour, physical organic chemistry underpins a range of fields and has wide application. As such, we have taken the approach for this conference that the area is a 'broad church' and encompasses not just the traditional physical organic areas of mechanism, reactivity and structure but extends into biology, materials science and systems chemistry. This breadth is represented by the range of presentations and the three streams of the conference.

- Physical Foundations of Organic Reactivity
- Mechanism and Bioorganic Chemistry
- Supramolecular and Systems Chemistry

We are thrilled that this approach has seen a particularly strong response worldwide, with more than 300 registered attendees from 35 countries and every (permanently inhabited!) continent.

A big "Thank you" is due to all participants, committee members, sponsors and (particularly) the student helpers for their efforts in making this conference a very successful event.

Once again, welcome to Sydney and enjoy the adventure-rich city and its picturesque surroundings.

### Jason Harper and Pall Thordarson Co-Chairs

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### **Organising Committee**

Co-Chair: Assoc. Prof. Jason Harper, University of New South Wales
Co-Chair: Assoc. Prof. Pall Thordarson, University of New South Wales
Dr Jonathon Beves, University of New South Wales
Prof. Stephen Blanksby, Queensland University of Technology
Prof. Michelle Coote, Australian National University
Prof. Katrina Joliffe, University of Sydney
Prof. Jonathan White, University of Melbourne

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### **UNSW Support Team**

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Varvara Efremova	Sinead Keaveney	Adam Martin	Muhammad Zenaidee
Abbas Farahani	Aaron Kennedy	Alex Mason	
Maurice Frerejean	Nicholas Konstandaras	Freya Mearns	

### **General Information**

### Address of Venue:

University of New South Wales (for more details see maps to follow).

### For emergencies please call:

+61 2 9385 6666 (UNSW Security Services)
+61 2 9385 4692 (Assoc. Prof. Jason Harper)
Emergency Services (Fire, Police, Ambulance) are reached by dialling 000.

### **Medical Services:**

UNSW Health Service Ground Floor East, Quadrangle Building (Grid Ref. E16) +61 2 9385 5425

### **Internet Access:**

Wifi internet access will be available at UNSW throughout ICPOC23. One option is the eduroam network - if you are familiar with and use this, this is likely most straightforward. If you do not use eduroam, there is a guest Wifi account set up for ICPOC23. Participants can click the link below and enter the event passphrase (which is ICPOC) and will be e-mailed a unique login. Note that it is strongly advised that you do this before you set off on your trip!

https://adguest.unsw.edu.au/request/retreive/8F4W5Ogro32333831g.XE9Z0ip

### **Conference App**

ICPOC23 has its own app, available from the Apple Store and Google Play, along with a web version. Either search the provider's stores for "ICPOC23" or use the links below (recommended for iPads, Macs).

- iPhone: https://itunes.apple.com/app/id1122604852
- Android: https://play.google.com/store/apps/details?id=com.attendify.confi4ykm7
- WebApp: http://i4ykm7.m.attendify.com/

Above and to the right is the QR code that can be used to download the app.



### Logo Design:

awooga, 35 Woodland Street, Marrickville, NSW 2034, Australia. awooga@iinet.net.au



### **Instructions for Presenters**

### **Oral Presentations**

PCs with Microsoft Powerpoint will be available in the venues. If you intend to use the provided equipment, please ensure that you bring your files on a USB flash drive and liaise with our AV helpers immediately *prior* to your session, to ensure that your presentation is ready at the start of the session.

Alternatively, you can connect your own computer to the projectors. Both HDMI and VGA connectors are available but please ensure that you bring any adapters that you might need. Once again, please test the connection with the aid of our AV helpers in the break immediately *prior* to your session starting.

Please ensure that you keep to your allocated time. There is no additional time for questions and discussion, so all presenters should allow time for discussion after their presentation. The presentation times will be rigorously enforced by the chairpersons!

### **Poster Presentations**

Posters will be presented in two sessions; authors are requested to mount their posters on the afternoon of the appropriate session (during the coffee break; you may choose to leave your posters at the registration desk and they will be mounted for you). The poster boards will be marked with the poster IDs; please attach your poster in the appropriate slot. Authors are assigned to the poster sessions as follows:

- Poster Session 1 (Tuesday 5<sup>th</sup> July): Authors' last names **A through L**.
- Poster Session 2 (Thursday 7<sup>th</sup> July): Authors' last names **M through Z**.

Authors are expected to be near their posters during the allocated poster sessions to allow discussion. Beverages and finger food will be provided during the poster sessions.

The maximum poster size is A0 (841 x 1189 mm). The poster boards can only fit A0 posters in the portrait orientation. Hence, while the posters do not have to be A0 in size, the maximum width is 841 mm. Material for handling posters will be provided.

Please remove your posters after your assigned poster session. Any posters still mounted at the end of the session will be removed.

There will be several **poster awards**, which will be decided on during the poster sessions. The awardees will be announced in the closing remarks on Friday 8<sup>th</sup> July.

### ICPOC23 App: Helpful Tips

### **Search filters**

The Detailed Program contains information about all planned events, such as presentations and posters. In this menu, choosing the search option, then the filter icon, highlights the events relevant to your interests. Filter results by stream, keynote lectures and even social events.



Details	Details		
Plenary Lectures	Location Leigthton Hall Scientia - tap for location		
Arieh Warshel (PL1 - Nobel Prize in Chemistry 2013): How Do	Location     PL1 (Scientia - Sunday)		
They Not Work: Advances in	DESCRIPTIØN		
Simulations and Computer Aided Enzyme Design © 320 pm - 425 pm	Plenary lecture. Prof. Arieh Warshel, Nobel Prize in Chemistry 2013. Session chair: Prof. Michelle Coote.		
Scientia - Leighton Hall	PRESENTERS		
DESCRIPTION	Arieh Warshel Prof. University of Southern Californi		
PRESENTERS +	+		
DOCUMENTS	DOCUMENTS		
Home Bookmarks Notes Search	Home Bookmarks Notes Search		

### Bookmarks

Note important information in one easy place. Tap the + to save speakers, events, campus locations and sponsors in your bookmarks.

### Reminders

Create a tailored schedule by tapping the + next to a session in the Detailed Program. This brings up reminder options for 10, 30 or 60 minutes before the event. Reminders are saved in Bookmarks, under Detailed Program.



# Map of the University of New South Wales





### ICPOC23 - Map of venues - UNSW, Sydney

### **Programme at a glance – Sunday 3<sup>rd</sup> July**

	Sunday 3rd July			
1:00 PM	Registration (Venue: John Niland Scientia Building)			
	Introductory Session - Chair: Harper (Venue: Leighton Hall)			
3:00 PM	Introductory Remarks -			
3:05 PM	Harper			
3:10 PM	Formal welcome -			
3:15 PM	UNSW Representative			
	Plenary Session 1a - Chair: Coote (Venue: Leighton Hall)			
3:20 PM	PL1 - Warshel			
	How Do Enzymes Work and How Do They Not Work: Advances in Simulations and Computer Aided Enzyme Design			
	Plenary Session 1b - Chair: Thordarson (Venue: Leighton Hall)			
4:25 PM	PL2 - Whitesides			
	Water, the Hydrophobic Effect, Entropy/Enthalpy Compensation, and Molecular Recognition in Biochemistry			
5:30 PM				
6:00 PM	Welcome Reception			
	Venue: Tyree Room			

### **Programme at a glance - Monday 4<sup>th</sup> July**

		Monday 4th July			
	Plenary/Keynote Session 2 - Chair: Echegoyen (Venue: CLB7)				
9:00 AM		PL3 - Campos (JPOC Award Lecture) How Roy G. Biv Evicts Two Triplets			
0.50 414		KI1 Darkor			
9.30 AW	Twisting tails and curious channe	els deliver both reaction chemistry and allostery	for the phosphoribosyltransferase		
10:20 AM		KL2 - Scott			
	Growi	ng Carbon Nanotubes From Synthetic Organic Er	nd-Caps		
10:50 AM		Coffee Break			
		Parallel Sessions 1			
	Physical Foundations	Bioorganic and Mechanism	Supramolecular and Systems		
11:20 AM	ILA1 - Ess	ILB1 - Pischel	ILC1 - Clever		
11120 /					
11:40 AM	CLA1 - Al-Shammary	CLB1 - Laws	CLC1 - Officer		
11:55 AM	ILA2 - Chan	ILB2 - Cristiano	ILC2 - Bures		
12:15 PM	CLA2 - Gryn'ova	CLB2 - Keaveney	CLC2 - Berry		
12:25 PM	ILA3 - Coote	ILB3 - Pavez	ILC3 - Smith, B.		
12:45 PM	A CLA3 - Meyer CLB3 - Tadgell		CLC3 - Del Guerzo		
12:55 PM					
1:00 PM	Lunch Break				
	Plenary/Keynote Session 3 - Chair: Beves (Venue: CLB7)				
2:00 PM	PL4 - Huang Nanostructures Prepared from Self-Assembly of Pillararene-Based Amphiphiles and Supra-Amphiphiles				
2:50 PM	KL3 - Kamerlin				
	Phosphoryl and Sulfuryl Transfer Reactions: Challenges in Interpreting Experimental and Theoretical Data				
3:20 PM	KL4 - Echegoyen				
	Are Fullerenes E	Effective AntiHIV Agents? Recent Results and Me	chanistic Studies		
3.20 DM		Coffee Break			
5.501101		Parallel Sessions 2			
	Physical Foundations	Bioorganic and Mechanism	Supramolecular and Systems		
	Chair: Yamazaki (Venue: CLB6)	Chair: Glover (Venue: CLB7)	Chair: Wilkinson (Venue: CLB8)		
4:20 PM	ILA4 - Trevitt	ILB4 - Yates	ILC4 – Garcia-Rio		
4:40 PM	CLA4 - Bucher CLB4 - Chung CLC4 - Rawa		CLC4 - Rawal		
4:55 PM	ILA5 - Rijs	ILB5 - Kyne	ILC5 - Moorthy		
5:15 PM	ILA6 - Blanksby ILB6 - Buurma ILC6 - Herges		ILC6 - Herges		
5:35 PM	CLA5 - Usui	CLC5 - Sperger	CLC5 - Bhosale		
5:45 PM					
5:50 PM					
6:30 PM	White House Pizza & Drinks				

### **Programme at a glance – Tuesday 5<sup>th</sup> July**

	Plen	Tuesday 5th July	<b>1 R7</b> )		
9:00 AM	PL5 - Mayr				
	Philicities, Fugalities, and Equilibrium Constants				
9:50 AM	KIS-O'Dopodhue				
51007.001	Umpolung Acy	I-Anion Catalysis by Carbenes: Understanding Ch	nemoselectivity		
10:20 AM	P-Cher	KL6 - Lammertsma nistry — From P4 to P-Ligands to P-polymer to P-c	chirality		
10:50 AM		Coffee Break			
	Physical Foundations	Bioorganic and Mechanism	Supramolecular and Systems		
	Chair: Humeres (Venue: CLB6)	Chair: Cristiano (Venue: CLB7)	Chair: Metrangolo (Venue: CLB8)		
11:20 AM	ILA7 - Johnson	ILB7 - Kurti	ILC7 - Andreasson		
11:40 AM	CLA6 - Kronja	CLB6 - Thongpanchang	CLC6 - Martin		
	-				
11:55 AM	ILA8 - White	ILB8 - Amedjkouh	ILC8 - Wilkinson		
12:15 PM	CLA7 - Scotson	CLB7 - Lee, R.	CLC7 – Brea-Fernandez		
12:25 PM	ILA9 - Williams, C.	ILB9 - LaCour	ILC9 - Webb		
12:45 PM	CLA8 - Glaser	CLB8 - Peng, Q.	CLC8 - Tu		
1:00 PM	Lunch Break				
2.00 DM	Pler	hary/Keynote Session 5 - Chair: White (Venue: C	:LB7)		
2:00 PIVI	Rationally Designed Biomimetic Polymers for Protein Stabilization and Delivery				
			-		
2:50 PM	Mass	KL7 - Pan Mass Spectrometric Study of Occuric Departice Internet distant			
	101033	spectrometric study of organic heactive interne			
3:20 PM		KL8 - Williams, S.			
	Diss	ecting the mechanisms of endo-acting mannosic	lases		
3:50 PM		Coffee Break			
		Parallel Sessions 4			
	Physical Foundations Bioorganic and Mechanism Supramolecular and Systems				
4:20 PM	ILA10 - Yamazaki	ILB10 - Satoh	ILC10 - Reimers		
4:40 PM	CLA9 - Wagner	CLB9 - Alabugin	CLC9 - Croft		
4:55 PM	VI ILA11 - Kable ILB11 - Wille		ILC11 - Smith, D.		
5:15 PM	ILA12 - Bieske ILB12 - Bottle ILC12 - DiLabio		ILC12 - DiLabio		
		CI-D10 Jacquer	CI C10, Constan Correio		
5:35 PIVI	CLATO - NAKATA	CLBIO - Jaeger	CLCTO - Sanchez-Garcia		
5:50 PM	Flash Posters	Flash Posters	Flash Posters		
6:00 PM	Poster Session				
		Venue: Tyree Room			
0.00 044					

### **Programme at a glance – Wednesday 6<sup>th</sup> July**



### **Programme at a glance – Thursday 7<sup>th</sup> July / Friday 8<sup>th</sup> July**

	Plen	Thursday 7th July ary/Keynote Session 7 - Chair: Faston (Venue: (	CLB7)		
9:00 AM	PL7 - Flitsch Enzyme Cascades for the Stereoselective Synthesis of Organic Compounds				
9:50 AM		KL11 - Abe π-Single Bonded Species			
10:20 AM	Hidden Entrop	KL12 - Evstigneev ic Contribution In Thermodynamics Of Molecula	r Complexation		
10:50 AM		Coffee Break			
L		Parallel Sessions 7			
	Physical Foundations Chair: Wille (Venue: CLB6)	Bioorganic and Mechanism Chair: de Voss (Venue: CLB7)	Supramolecular and Systems Chair: Escuder (Venue: CLB8)		
11:20 AM	ILA18 - Uggerud	ILB18 - Easton	ILC18 - Metrangelo		
11:40 AM	CLA12 - Marshall	CLB12 - Laos	CLC12 - Ulatowski		
11:50 AM	ILA19 - Gudmundsdottir	ILB19 - Payne	ILC19 - Pfeffer		
12:10 PM	CLA13 - Streubel	CLB13 - Ainsworth	CLC13 - Cockroft		
12:20 PM		CLB14 - Britton			
12:30 PM	CLA14 - Espinosa Feroa	CLB15 - Chatterjee	CLC14 - Cao		
12:40 PM	ILA20 - Sander ILB20 - Barrow ILC20 - von Delius		ILC20 - von Delius		
1:00 PM	Lunch Break				
-	Plenar	y/Keynote Session 8 - Chair: Thordarson (Venue	e:CLB7)		
2:00 PM	PL8 - van Esch Out-of-Equilibrium Biomimetic Supramolecular Architectures by Dynamic and Dissipative Self-Assembly				
2:50 PM	KL13 - Corminboeuf Finding DORI: a multifaceted tool built upon chemical bonding				
3:20 PM	KL14 - Pross The Persistence Principle: Seeking to Reconcile Boltzmann and Darwin				
3:50 PM	Coffee Break				
•	Physical Foundations Chair: Croft (Venue: CLB6)	Parallel Sessions 8 Bioorganic and Mechanism Chair: Buurma (Venue: CLB7)	Supramolecular and Systems Chair: Pfeffer (Venue: CLB8)		
4:20 PM	ILA21 - Ho	ILB21 - Glover	ILC21 - Jolliffe		
4:40 PM	CLA15 - Jones	CLB16 - Kumar	CLC15 - Reany		
4:55 PM	ILA22 - Wilson ILB22 - Raston		CLC16 - Badijic		
5:10 PM 5:15 PM	CLA16 - Gbayo CLB17 - Wang, X.		CLC17 - Wen		
5:25 PM	ILA23 - Yu, ZX. ILB23 - Humeres		ILC22 - Day		
5:45 PM	CLA17 - Doughty	CLB18 - Legault	CLC18 - Gloe		
6:00 PM	Flash Posters	Flash Posters	Flash Posters		
6:10 PM	Posters Posters Posters				
8:30 PM					

### **Programme at a glance – Friday 8<sup>th</sup> July**

Friday 8th July

Keynote Session 9 - Chair: Jolliffe (Venue: CLB7)



### Forum on the Future of Chemistry @ UNSW - 6<sup>th</sup> July 2016

UNSW John Niland Scientia Building – Tyree Room, 4 -6 pm.

### **Opening address: Prof. George Whitesides – Harvard University**

### Panel members:

George Whitesides	Prof. Harvard University.
Andrew Holmes	President of the Australian Academy of Science, Prof. School of Chemistry, University of Melbourne.
Peter Götlitz	Editor-in-Chief of Angewandte Chemie, Wiley-VCH.
Justin Gooding	Deputy Head, School of Chemistry, University of New South Wales, co-chair of the Australian Nanomedicine Centre, ARC Laureate Fellow.
Veena Sahajwalla	Director SMaRT@UNSW, Associate Dean Strategic Industry Relations – Science, University of New South Wales, ARC Laureate Fellow.
Peter Junk	President Elect of the Royal Australian Chemical Institute (RACI), Professor, James Cook University Townsville.

MC: Assoc. Prof. Pall Thordarson, University of New South Wales.

### Attendance is free!

### Everyone interested in the Future of Chemistry is welcome.

The panel discussion will run in Q&A format with plenty of opportunities for the audience to contribute to the discussion. Light refreshments will be provided before and after the event. While not necessary, to help us planning / catering we encourage you to register your interest at the link below.

https://www.surveymonkey.com/r/XD7TVCC

*Event organisers:* School of Chemistry and the Faculty of Science, University of New South Wales, Systems Chemistry Australia and 23<sup>rd</sup> IUPAC Conference on Physical Organic Chemistry.

### **Sponsors**

- Angewandte Chemie International Edition (Wiley-VCH)
- Royal Australian Chemical Institute (RACI)
- ARC Centre of Excellence in Bio-Nano Science (CBNS)









### **Conference Excursion - 6<sup>th</sup> July 2016**

Wednesday afternoon we will offer a **FREE cruise on Sydney Harbour for conference participants**. Included will be:

- Return coach transfers from the University of New South Wales, departing at *ca*. 1:45 pm and returning around 5:15 pm.
- Two hour private cruise around Sydney Harbour.
- Drinks and finger food will be provided on board

We encourage you to register your interest at the link below.

https://www.surveymonkey.com/r/XD7TVCC





### **Poster Presentations – Tuesday 5<sup>th</sup> July**

No.	Presenter	Institution	Title
TU1	Karma Albalawi	Cardiff University	Double competition dialysis: identification orthogonal recognition elements for nucleic acid templated nanostructures
TU2	Anuradha	RMIT University	Induction and controlled chiral supramolecular structures from hierarchical self-assembly of achiral compounds
TU3	Alexandra Daryl Ariawan	University of New South Wales	The cyclic peptide unguisin A is a selective anion receptor
TU4	Rabia Ayub	Uppsala University	A computational study of compounds with nonpolar "aromatic chameleons" character
TU5	Tae-Hyun Bae	Nanyang Technological University	Tailoring Crystalline Microporous Materials for Energy-Efficient Gas Separations
TU6	Anna Bielawska	Medical University of Bialystok	Biophysical aspects and biological implication on the interaction of novel alkyl pyridine platinum complexes with DNA
TU7	Krzysztof Bielawski	Medical University of Bialystok	Binding of octahydropyrazin[2,1-a:5,4-a']diisoquinoline derivatives to DNA: spectrofluorimetric analysis and molecular modeling studies
TU8	Jeffrey Black	University of New South Wales	Thermoelectrochemistry of Lithium-Glyme Solvate Ionic Liquids: Towards Waste Heat Harvesting
TU9	René-Chris Brachvogel	FAU University Erlangen-Nuremberg	Self-sorting of Orthoester Cryptates
TU10	Dong Wook Chang	Pukyong National University	Facile Solution-Based Synthesis of Nitrogen-Doped Graphene as Electrocatalysts for Oxygen Reduction Reaction
TU11	Harriet Clarke	University of Southampton	Anion transport and binding properties of NN'- (phenylmethylene)dibenzamide based receptors
TU12	James Cooper	University of Edinburgh	Study of Metallosupramolecular Complexes in Nanopores
TU13	Emily Crawley	Flinders University	Application of shear stress mediated refolding technology to the oxidative refolding of insulin
TU14	Kajetan Dąbrowa	Institute of Organic Chemistry PAS	Strategies for Synthesis of Unclosed Cryptands via H-Bond Templated Macrocyclization and Subsequent Mild Postfunctionalization
TU15	Nicholas Dominelli Whiteley	University of Edinburgh	The Energetic Limit of Cooperativity in H-bond Chains
TU16	Eric Du	University of New South Wales	Peptide hydrogel properties and cardiac stem cells.
TU17	Genevieve Duché	University of New South Wales	Combining liposomes and self-assembled peptide hydrogels for drug delivery and aesthetic therapy.
TU18	Morphy Dumlao	University of New South Wales	Internal energies of benzylammonium ions formed by low temperature plasma mass spectrometry: Effects of different ionisation waveforms on molecular ion survival, ionisation efficiency, and power consumption

No.	Presenter	Institution	Title
TU19	Daniel Fankhauser	Australian National University	Chiral Organic Hosts in Asymmetric Reactions
TU20	Abbas Farahani	University of New South Wales	Effect of Aromatic Capping Group on Packing of Amino Acids
TU21	Thomas Garrard	University of Melbourne	Ionic-liquid supported hydrogen atom transfer reagents: synthesis and kinetics
TU22	Nadine Gass	Karlsruhe Institute of Technology	Exploration of Benzophenone nucleosides for photocatalytic DNA
TU23	Alyssa Gilbert	University of New South Wales	Identifying ionic liquid effects on the rate constant of an $S_{\rm N}1$ process
TU24	William Hart	University of New South Wales	Fractionation of lignin through the use of ionic liquids
TU25	Md. Musfizur Hassan	University of New South Wales	Rational and Strategic Design of Hydrogelators for Controlled Drug Delivery
TU26	Rebecca Hawker	University of New South Wales	Rational selection of the cation of an ionic liquid solvent to control the reaction outcome of an SN2 process
TU27	Robert Healey	University of New South Wales	Tag-specific and residue-specific fluorescent labelling of a GPCR protein drug
TU28	Celine Heu	University of New South Wales	The relationship between structure, biocompatibility, local and bulk rheological properties in self-assembled hydrogels for <i>in vitro</i> 3D cellular models
TU29	Tomoya Ichino	Hokkaido University	Theoretical Study on Organocatalytic Diboration of Pyrazines: Radical– Mediated Catalytic Reaction
TU30	Laura Jowett	University of Southampton	Anion Transport Properties of Perenosins for Potential Anti-Cancer Therapy
TU31	Daisuke Kaneno	Kochi University	Diastereoselectivity and Reactivity of the Hydroboration of Allylic Substituted Alkenes
TU32	Mehdi Khalaj	Islamic Azad University	Synthesis, characterization, antibacterial and catalytic activity of nanopolymer supported copper (II) complex as a highly active and recyclable catalyst for the formamidation of arylboronic acids under aerobic conditions
TU33	Tae Oh Kim	Kumoh National Institute of Technology	Improved the Performance of DSSCs accomplished by Composition of Zr/N doped TiO2
TU34	Tae Oh Kim	Kumoh National Institute of Technology	High performance of DSSCs accomplished by composition of graphene/N doped TiO2 electrodes
TU35	Bonghyun Kim	Seoul National University	Aminopeptidase N (APN) inhibitors and analogs from a novel chiral synthon
TU36	Young-seok Kim	Korea Electronics Technology Institute	Electrically Tunable Photonic Crystals Device with High Cyclic Stability

No.	Presenter	Institution	Title
TU37	Young-seok Kim	Korea Electronics Technology Institute	Anti-corrosion Property of Graphene based Coating Material
TU38	Paul King	University of Sydney	The Mechanism of the Oxa-Pictet-Spengler Reaction
TU39	Nicholas Konstandaras	University of New South Wales	Correlating structure and reactivity: Electronic and strain effects in a range of systems
TU40	Li-Ting Lee	Feng Chia University	Novel Ternary Blends with Chemically Hydrogen-bonding Interactions
TU41	Hyun Eui Lee	University of New South Wales	Capturing Reactive High-Valent Iron (IV)-oxo Intermediates of Catalytic Cycles using Theta-capillary Nanoelectrospray Ionisation
TU42	Wei Lin Leng	Nanyang Technological University	Stereoselective <i>C</i> -Glycosylation: Pd- and Ir-catalyzed Decarboxylative Allylation of Glycals and Amino Alkanoic Acids
TU43	Chunju Li	Shanghai University	Synthesis of a Water-soluble Carboxylatobiphen[4]arene and Its Complexation Towards Paraquat
TU44	Ian Lin	University of New South Wales	Impact of Increasing Hydrophilicity on Hydrogel Biocompatibility
TU45	Miroslav Ludwig	University of Pardubice	Tuning Two-Photon Absorption Cross-Section in Model Push-Pull Chromophores
TU46	Anna Lundstedt	Uppsala University	Ozonolysis of polycyclic aromatic hydrocarbons in participating solvents
TU47	Chin Ken Wong	University of New South Wales	Non-spherical polymersomes obtained through fine-tuning of $\pi$ -stacking strengths in perylene-containing diblock terpolymers

### **Poster Presentations – Thursday 7<sup>th</sup> July**

No.	Presenter	Institution	Title
TH1	Neil Mallo	University of New South Wales	Photoswitchable molecular devices
TH2	Alex Mason	University of New South Wales	Di- and tri-block copolymers synthesized by SET-LRP that self-assemble in water to form polymersomes with asymmetric membranes
TH3	Ildikó Móczár	Budapest University of Technology and Economics	5,5-Dioxophenothiazine-based chiral anion sensors
TH4	Joses Grady Nathanael	University of Melbourne	Oxidative Damage of Small Peptides by the Air Pollutants NO <sub>2</sub> <sup>•</sup> and NO <sub>3</sub> <sup>•</sup>
TH5	Michael Nordlund	Uppsala University	Organometallic Fullerene Derivatives:Synthesis of a Ferrocene-[60]Fulleropyrrolidine Trimer
TH6	Sandra Olsson	Uppsala University	Design of porphyrin host-guest systems for determination of relative stereochemistry
TH7	Henrik Ottosson	Uppsala University	The cyclopropyl group: an aromaticity indicator in the first triplet and singlet excited states
TH8	YoonKook Park	Hongik University	Interactions energies of tetraalkylphosphonium cation and amino acid anion based ionic liquids in gas phase
TH9	Hoyyul Park	Korea Electrotechnology Research Institute	Thermally Curable Silica-Epoxy Hybrid Materials Using Organically Modified Various Sized Silica Nanoparticles and Methyl-Glycidyl Oligosiloxanes
TH10	Qiuli Qi	The Chinese University of Hong Kong	Host-Guest Binding Properties of Di(amide-triazole)s Containing Two Anion Binding Sites
TH11	Mr Lei Qin	School of Chemistry, The University of Sydney	Macrocyclic Squaramides: Anion Receptors with High Sulfate Binding Affinity and Selectivity in Aqueous Media
TH12	Anushri Sopan Rananaware	RMIT University	Tetraphenylethene-based derivatives for supramolecular self- assembly
TH13	Lisa Randone	Australian National University	Towards Construction of Insulated Molecular Wires by Crystal Engineering of Cyclodextrin-based Rotaxanes
TH14	Andrew Robinson	University of New South Wales	The Effect of Polarity and Chirality on the Properties of Self- assembled Peptide Hydrogels
TH15	David Rombach	KIT Karlsruhe	Photoredox catalysis using polystyrene supported Ru(bpy) <sub>3</sub> Cl <sub>2</sub> and perylene bisimide-based photoredox catalysts
TH16	Kenichiro Saita	Hokkaido University	Theoretical study on mechanism of the photochemical ligand substitution of fac-[ReI(bpy)(CO)3(PR3)]+ complex
TH17	Karin Schaffarczyk McHale	University of New South Wales	Investigating microscopic interactions to explain ionic liquid effects in bimolecular nucleophilic substitution processes
TH18	Christian Schwechheimer	Karlsruhe Insitute of Technology	Synthesis, Spectroscopic Studies and Applications of Novel Cyanine-Styryl Dyes

No.	Presenter	Institution	Title
TH19	Narges Shamsaei Zafarghandi	Melbourne University	Greener Approaches To Radical Chemistry: An investigation of the fundamental reactivity of carbon centred radicals in ionic liquids
TH20	Yasuhiro Shigemitsu	Nagasaki University	Enhanced Sampling Analysis for the Free Energy Surface using Reax Force Field : Weak Solute and Solvent Coupling Cases
TH21	Yukihide Shiraishi	Tokyo University of Science Yamaguchi	Hybrid Thermoelectric Materials Composed of CNT/Pd Nanoparticles/Poly(vinyl chloride)
TH22	Ratnanjali Shrivastava	Dayalbagh Educational Institute	A Novel Graphene/Chitosan/ZrO2 nanocomposite sensor for electrochemical investigation of a non-steroidal anti- inflammatory drug Tolfenamic Acid
TH23	Michael Spooner	University of Southampton	Trans-membrane Anion Transport – Uncovering the Rules that Govern Transporter Efficiency
TH24	Yosuke Sumiya	Hokkaido University	Kinetic Analysis for Complex Reaction Networks: Importance of Conformational Entropy
TH25	Bethany Taggert	University of Melbourne	Gas-Phase Studies of Radical-Mediated Polymer Fragmentation
TH26	Yong Chua Teo	National Institute of Education, Nanyang Technological University	Indium-Catalyzed C(sp <sup>3</sup> )-H Functionalization of 2- Methylazaarenes through Direct Benzylic Addition to Trifluoromethyl <sub>Ketones</sub>
TH27	Dasan Thamattoor	Colby College	An Experimental and Computational Investigation of (a- Methylbenzylidene)carbene
TH28	Dasan Thamattoor	Colby College	Photochemical Generation of Strained Cycloalkynes from Methyleneyclopropanes
TH29	Pall Thordarson	University of New South Wales	Open Data Fit – Open Access to Physical Organic Chemistry Data
TH30	Kristel Tjandra	University of New South Wales	Synthesis of Multivalent Peptide Scaffold for the Targeting of Cancer Cells
TH31	Ruibing Wang	University of Macau	Encapsulation of Camptothecin by Cucurbit[7]uril: Reduced Toxicity with Preserved Anti-Cancer Activity
TH32	Xinchang Wang	Xiamen University	Assembled molecular face-rotating polyhedra to transfer chirality from two-dimensional to three-dimensional
TH33	Huixin Wang	University of New South Wales	High and Low Energy Collision Induced Dissociation of Supercharged Protein Ions formed by Electrospray Ionization
TH34	James Webb	University of New South Wales	Ultra-Fast Energy Transfer in Fluorescent Perylene Arrays
TH35	Jonathan Wojciechowski	University of New South Wales	Designing Supramolecular Heat-Set Hydrogels for 3D Cell Culture
TH37	Yang Xiao	University of Wollongong	Developing Photoacids for Chemopropulsion
TH38	Shohei Yoshidomi	Hiroshima University	Nitrogen Atom Effect on the Reactivity of Localized Singlet Diradicals

No.	Presenter	Institution	Title
TH39	Ying Yu	South China Normal University	Detection of Phosmet Residues Using a Fluorescent Probe Base on Supramolecular Effect
TH40	Li-Ming Yuan	Yunnan Normal University	Vancomycin Enantioselective Membrane for Separation of 4- Hydroxy phenylglycine
TH41	Qingshu Zheng	The University of Edinburgh	Understanding Aurophilic Interactions
TH42	Yongbin Zhuang	Xiamen University	Computational study on narcissistic chiral self-sorting of face-rotating organic polyhedra
TH43	Vincent E. Zwicker	University of Sydney	Linear zinc(ii)dipicolylamine-functionalised peptides as highly selective pyrophosphate sensors in physiological media
TH44	Catherine Jessica Onie	University of New South Wales	Influence of Alkyl Chain Length and Anion Species on Ionic Liquid Structure at the Graphite Interface as a Function of Applied Potential
TH45	Muhammad Zenaidee	University of New South Wales	Extreme protein supercharging: Profiling the pH of electrospray generated droplets and improving ion fragmentation