

**71st Irish Universities Chemistry Colloquium jointly hosted by
Technological University Dublin and RCSI
on the 20th and 21st June 2019**

Thursday 20th June, 2019

Technological University Dublin, City Campus, Aungier St

8:30	Registration: Main Entrance TU Dublin, Aungier Street	
9:00	Welcome Address Prof Declan McCormack - Head of School, Chemical & Pharmaceutical Sciences, TU Dublin, City Campus Room 4027 (4 th Floor) TU Dublin, Aungier Street	
9:15	Plenary 1 Prof. Luuk Van der Wielden (UL) Room 4027 (4 th Floor) TU Dublin Aungier Street	
	Room 4068	Room 4079
	Session 1A: Organic Chemistry Chair: Dr Grainne Hargaden	Session 1B: Physical & Analytical Chemistry Chair: Dr David O'Connor
10.00	Speaker 1 <i>Synthesis of tail Fragment Analogues of Nisin, A bacteriocin peptide.</i> W. Travers (TU Dublin, Tallaght)	Speaker 2 <i>Quantitative resazurin assay of cell viability for release alkaline phosphatase (ALP)</i> Thanih Balbaied (UCC)
10.20	Speaker 3 <i>Recent Advances in the Synthesis and biological Application of ferrocenyl derivatives.</i> K.Ontiveros (DCU)	Speaker 4 <i>Franck-Condon Calculations of the Q-band Absorption of Phthalocyanines</i> Kevin McGuire (NUI Maynooth)
10.40	Flash Talks Session 1 F1: C. Cioffi (RCSI) F2: G. Palop (NUIG) F3: R Kruschel (UCC) F4: S. Kavanagh (UCD)	Flash Talks Session 2 F5: P. McNeice (QUB) F6: M. Haskins (UL) F7: M. Craig (TCD) F8: P. Sidambaram (TU Dublin, City Campus)
11.00	Coffee and Poster Session 1 Room 5050	
	Room 4068	Room 4079
	Session 2A: Inorganic & Materials Chemistry Chair Dr Ariane Perez-Gavilan	Session 2B: Physical & Analytical Chemistry. Chair: Dr Eoin McGillicuddy

11.45	<p>Speaker 5 <i>Enhancing the bioavailability of drugs through cocrystallization and coamorphization</i> M. Aljohani (NUIG)</p>	<p>Speaker 6 <i>Defect modelling of LaGaO₃ for solid oxide fuel cell applications</i> J. Savioli (TCD)</p>
12.05	<p>Flash Talks Session 3 F9: A. Mahon (UCD) F10: S. O'Halloran (DCU) F11: T. Xie (QUB) Barry Reid GPE Scientific</p>	<p>Flash Talks Session 4 F12: F. O'Maolmhuaidh (DCU) F13: F. Muraca (UCD) F14 M. Lynch (UCC)</p>
12.25	Lunch	
2.00	<p>Panel discussion Where to Now? A Roundtable Discussion With Academic Funders And Industrial Experts Room 4068</p>	
	Room 4068	Room 4079
	<p>Session 3A: Organic Chemistry Chairs: Prof. C. Marmion & Prof. John Cassidy</p>	<p>Session 3B: Inorganic & Materials Chemistry Chair: Dr John Colleran</p>
2.45	<p>Speaker 7 ICI postgraduate Award Winner 2018 Adele Gabba (NUIG)</p>	<p>Speaker 8 <i>Multifunctional Hydrogels – A novel approach to Interpenetrating Networks</i> S. Bolanta (UL)</p>
3.05	<p>Speaker 9 <i>Biotransformations employing nitrile hydrolyzing enzymes towards the enantioselective synthesis of β-amino acids</i> T. Mareya (WIT)</p>	<p>Speaker 10 <i>Manganese Coordination Complexes: From Aesthetically Pleasing Geometries to Biological Mimics</i> S. Tandon (TCD)</p>
3.25	<p>Speaker 11 <i>Development of an Asymmetric Synthesis of Ergoline Derivatives</i> R. Connon (UCD)</p>	<p>Speaker 12 <i>Plasmon-Mediated Visible-Light-Driven Conversion of CO₂ over RuO₂/TiO₂ Catalysts</i> E. Morais (UCD)</p>
3.45	<p>Coffee and Poster Session 2 Room 5050</p>	

<p>4.05</p>	<p>Flash Talks Session 5 F15 F. Alletto (RCSI) F16: F. Meany (NUIG) F17: K. Tseke (WIT)</p>	<p>Flash Talks Session 6 F18: H. Jenkins (TU Dublin, Tallaght) F19: I.F. Robayo Molina (UL) F20: D. Mulrooney (UCD) F21: Graham M Reid (UCD)</p>
<p>4.25</p>	<p>Speaker 13 <i>Asymmetric Copper-Catalysis used for Efficient Desymmetrisation in Intramolecular C–H Insertion Reactions of α-Diazo-β-oxo Sulfones</i> T. Brouder (UCC)</p>	<p>Speaker 14 <i>A Salt free method for preparing stable Au/Ag aggregates as liquid SERS substrates for the detection of biomolecules under difficult conditions</i> Z Ye (QUB)</p>
<p>4.45</p>	<p>Speaker 15 <i>Influence of Substituents on Aggregation in a series of mono and diamide isomers</i> I. Osman (DCU)</p>	<p>Speaker 16 <i>The Development of Metal Complexes of the Hedgehog Pathway Inhibitor GANT61-D as Potential Anticancer Agents</i> A.Ryan (RCSI)</p>
<p>5.05</p>	<p>Speaker 17</p>	<p>Speaker 18 <i>Carrier profiling in molecular layer doped Si nanowires: effects of the density and width of the nanowires</i> Margarita Georgieva (CIT)</p>
<p>6.00</p>	<p>Barbeque Odeon, Harcourt St</p>	

Friday 21st June, 2019

Royal College of Surgeons of Ireland

Houston lecture Theatre	
9.15	Opening & Welcome to RCSI Prof Donal O'Shea Head of Department of Chemistry RCSI
	Session 4: Inorganic & Materials Chemistry Chair: Dr. Darren Griffith
9.30	Speaker 19 <i>Synthesis and Design of new type 3 porous liquids</i> J. Cahir (QUB)
9.50	Speaker 20 <i>Investigation of Phosphine based Ligands for the Synthesis of Inorganic CsPbX₃ Nanocrystals</i> Fiona McGrath (UL)
10.10	Speaker 21 <i>An experimental and kinetic modelling study on oxidation of diisobutylene</i> N. Locachari (NUIG)
10.30	Speaker 22 <i>Copper ferrite (CuFe₂O₄) as a catalyst in CuAAC</i> Bartlomiej Wojciechowski (TU Dublin City Campus)
10.50	Coffee: 1784 Restaurant Tour: <i>History and Location of First Chemistry Teaching and Research in Ireland</i> (11.05 optional)
	Session 5A: Organic Chemistry Chair: Prof. Mauro Adamo
11.20	Speaker 23 <i>3D Printing of Spatially Patterned Magnetically Responsive Hydrogels</i> P.Monks (RCSI)
11.40	Speaker 24 <i>Glycocomimetics to Inhibit Candida Albicans Adhesion</i> H.Martin (NUIM)
12.00	Plenary 2 <i>Continuous Flow biocatalysis for highly sustainable and versatile syntheses</i> Dr. Francesca Paradisi (The University of Bern)
12.45	Closing Session & Prize Giving

Flash talks listing.**The F number also refers to the poster number in the poster session**

No.	Title	Presenter	Affiliation	Page
F1	<i>Sulfide as Leaving Group: Stereospecific Bromination of Benzylic Phenyl Sulfides</i>	C. Cioffi	RCSI	
F2	<i>Macrocyclic N-carboxyanhydrides to achieve homogeneous monodisperse Collagen-type materials</i>	Guillermo Palop	NUIG	
F3	<i>Synthesis of Isoquinolinequinone N-oxides as Anticancer Agents organic pharma</i>	Ryan Kruschel	UCC	
F4	<i>Development for the Asymmetric Grignard Synthesis of Tertiary Alcohols</i>	Saranna Kavanagh	UCD	
F5	<i>Binary Alkoxide Ionic Liquids: Homogeneous and Heterogeneous Catalysts</i>	Peter McNeice	QUB	
F6	<i>Crystal Engineering of Dihydrogen Phosphate-Phosphoric Acid Cocrystals</i>	Molly Haskins	UL	
F7	<i>High-Throughput Screening of Molecular Water Splitting Catalysts</i>	Michael Craig	TCD	
F8	<i>Electrochemistry Investigation of Uptake of Bioinorganic Silver-based Drug</i>	P. Sidambaram	TU Dublin, City Campus	
F9	<i>Design, Synthesis and Biological Evaluation of Aromatic Lipoxin A₄ Analogues</i>	Aine Mahon	UCD	
F10	<i>Development of Superoxide Dismutase (SOD) Mimetic Microstructures using Two-Photon Polymerization (2PP) and Click Chemistry</i>	Sean O'Halloran	DCU	
F11	<i>UV-Light Triggering Bioactive Nitric Oxide Release from Amine-Functionalised Polymers</i>	Tianchao Xie	QUB	
F12	<i>Biocompatible Screen-Printed Electrodes: Cell Viability Investigations</i>	Fionn Ó'Maolmhuaidh	DCU	
F13	<i>A novel tissue culture platform for the long term assessment of nanomaterial fate</i>	Francesco Muraca	UCD	
F14	<i>Computational Investigation of the Clustering Behaviour of Isonicotinamide in Common Solvents</i>	Mark Lynch	UCC	

F15	<i>Desulfurative fluorination of benzylic phenyl sulfides: a mean to late-stage ¹⁸F-labeling</i>	Francesco Alletto	RCSI	
F16	<i>Study of substituents on the influence of a 2-O-benzoate group on the Lewis acid promoted anomeration of a glucopyranoside</i>	Fiach Meany	NUIG	
F17	<i>Development and Optimisation of a Continuous-flow Process for the Enantioselective Synthesis of 3-Substituted Oxindoles</i>	Kavnem Tseke	WIT	
F18	<i>Investigating the Cytotoxicity under Hypoxic and Normoxic Conditions of Copper-Based Complexes in both Cancer-derived and Normalised cell lines</i>	Hollie Jenkins	TU Dublin Tallaght	
F19	<i>Organisation and Photoreactivity of Self-Assembled Metalloporphyrin Aggregates at the Interface between Two Immiscible Electrolyte Solutions</i>	Iván F. Robayo Molina	UL	
F20	<i>multifunctional layered magnetic materials: 2-D magnetic coordination polymers</i>	David Mulrooney	UCD	
F21	<i>Production of Antibacterial Polymeric Materials</i>	Graham M Reid	UCD	

Listing of posters

No.	Title	Presenter	Affiliation	Page
P1	<i>Synthesis of Nisin Derivatives to Investigate their Antibiotic Properties</i>	Dean Winder	TU Dublin Tallaght	
P2	<i>The First Enantioselective Synthesis of Gingesulfonic Acids and Unequivocal Determination of their Absolute Stereochemistry</i>	Grazia Bencivenni	RCSI	
P3	<i>Deep-Sea Drug Discovery; The Isolation And Characterisation Of Potent Novel Anti-Inflammatory Glycolipopeptides</i>	Sam Afoullouss	NUIG	
P4	<i>Metal-Based Glycoconjugates for the Targeted Anticancer Chemotherapy</i>	Ioannis Titilas	NUIG	
P5	<i>NIR Osmium (II) polypyridyl probe with a therapeutic twist: disrupting the mitochondrial membrane potential for targeted therapy</i>	Karmel Gkika	DCU	
P6	<i>Investigation of Hosts for Type 2 Porous Liquids</i>	Francesca M. Alexander	QUB	
P7	<i>Optimisation and Scale-up of the β-Chloroacrylamide Process using Batch and Continuous Flow Methods</i>	Olga Dennehy	UCC	
P8	<i>Photo-induced Electron Transfer at Liquid-Liquid Interfaces for Solar Energy Conversion</i>	Kamil A. Cywinski	UL	
P9	<i>Coordination chemistry of 2-picoyl naphthalene diimide and bis-phthalimide ligands</i>	June Lovitt	TCD	
P10	<i>Stability Studies on the Hydrolysis of Antimicrobial Inorganic Tellurium(IV) complexes</i>	Kenneth D'Arcy	NUIM	
P11	<i>Conjugated Polymer Nanoparticles as A New Class of Fluorescent Probes based on Emission Anisotropy</i>	Zixu Zhao	UCD	
P12	<i>New Tetrazole-Based Compounds for Coating Medical Implants: Synthesis and Corrosion Studies</i>	Rónan McAteer	TU Dublin Tallaght	
P13	<i>Pyridine 5-hydroxytriazoles: a new class of potential ligands for drug discovery and catalysis</i>	Roberta Pacifico	RCSI	
P14	<i>Synthesis Towards Constrained Anti-Adhesive Sia(α2-3)Gal Glycomimetics</i>	Syl Byrne	NUIG	
P15	<i>Next Generation Antisense Therapeutics</i>	Brionna Mc Gorman	DCU	

P16	<i>CTAB as a Non-Adsorbing “Promoter” for the Self-Assembly of Charged Colloidal Nanoparticles at Liquid-Liquid Interfaces into Multi-Dimensional Arrays</i>	Li, Xinyuan	QUB	
P17	<i>Source apportionment of ambient carbonaceous aerosol in Ireland using a variety of analytical techniques</i>	Eimear Heffernan	UCC	
P18	<i>Supramolecular Isomers of [Zn(glycolate)(bipy)_{1.5}]_n</i>	Chenghua Deng	UL	
P19	<i>Synthesis, spectroscopic properties and aggregation behaviour of terpyridine functionalized building blocks</i>	Jason Delente	TCD	
P20	<i>Estrogen-Copper(II) complexes as targeted anticancer metal-based drugs</i>	Stephen Barrett	NUIM	
P21	<i>Continuous Flow Photorearrangement of Isoxazoles</i>	Cormac Bracken	UCD	
P22	<i>Polypeptide-based hydrogels for tissue engineering</i>	Shona O’Brien	RCSI	
P23	<i>Novel Zn and Mg MOFs based on azo-dicarboxylate ligands and their potential for drug delivery</i>	Ahmed Ahmed	NUIG	
P24	<i>Plasmonic fluorescent assay for molecular lipid membrane binding, permeation and dynamics of permeation.</i>	Agata Steplewska	DCU	
P25	<i>Porous Polymeric Materials for Active Pharmaceutical Ingredient (API) Delivery</i>	Hung-Jui Chen	QUB	
P26	<i>Ambident Reactivity of Enolates: The Last Stand for HSAB Theory?</i>	Kevin Sheehy	UCC	
P27	<i>Electrochemiluminescence of Heavy Metal Free Nanomaterials for Applications in Biosensing</i>	Siobhán O’Connor	UL	
P28	<i>Smart Anionophores: Stimuli-Responsive Anion Transport</i>	Luke Marchetti	NUIM	
P29	<i>Synthesis and Applications of Cyclic Sulfonamides</i>	Aisha Khalifa	UCD	
P30	<i>Effects of nanoparticle-corona’s glycoproteins and their glycan component on the macrophage uptakes of silica nanoparticles</i>	Ngoc Duong Trinh	RCSI	
P31	<i>Ion-Responsive Self-Immolative Linkers for Drug Delivery</i>	Liam Fitzgerald	NUIG	
P32	<i>An investigation of mycotoxin induced DNA damage in IPEC-J2 Porcine Intestinal Cells</i>	Asmita Thapa	DCU	

P33	<i>Star polymers and cross-linked star polymer model networks prepared by aqueous RAFT polymerization for drug/DNA delivery</i>	Gavin Irvine	QUB	
P34	<i>On-line Analysis of Organic Aerosols in Air</i>	Niall O'Sullivan	UCC	
P35	<i>C₂H₂/CO₂ Separation Studies of Pyrazole Ligand Derived Hybrid Ultramicroporous Materials</i>	Naveen Kumar	UL	
P36	<i>Directed Self Assembly of Near Infrared Fluorescence Responsive Nanoparticles and their use for Cellular Imaging</i>	Niamh Curtin	RCSI	
P37	<i>Intrinsic Properties of Nitric Oxide Binding to Hemin and Hemin Conjugates: A Theoretical Study</i>	Amir Abdo	NUIG	
P38	<i>Gas Chromatography-Mass Spectrometry Analysis of Bacterial Volatiles</i>	Shane Fitzgerald	DCU	
P39	<i>Ionic Liquid-Assisted Synthesis of Nanocatalysts for the Direct Conversion of CO₂ to Hydrocarbons</i>	Zara Shiels	QUB	
P40	<i>Pressing solids directly into sheets of plasmonic nanojunctions enables solvent-free surface-enhanced Raman spectroscopy</i>	Li, Chunchun	QUB	
P41	<i>Filling in the gaps: A comprehensive analysis of light transmission through void-filled inverse opal photonic crystal materials</i>	Alex Lonergan	UCC	
P42	<i>Rapid Profiling of Enteric Coated Drug Formulations via Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS)</i>	Niamh O' Mahony	UCC	
P43	<i>Electrochemical sensing of Lactose in Fermentation Process Monitoring</i>	Grace Halpin	NUIM	
P44	<i>Bio-conjugations In Flow for Drug Conjugates and Theranostic Imaging Agents</i>	Sheila Fitzgerald	RCSI	
P45	<i>Cyclometalated Ir(III) Complexes as Triplet Photosensitisers for Efficient Visible-Light Absorption</i>	Nidhi Arora	TCD	
P46	<i>Developing tools for pesticide detection and toxicity testing in agricultural soils</i>	Mathavan Vickneswaran	DCU	
P47	<i>The Control of Single Nanowire Device's Electrical Performance via Seed Mediated Doping and Contact Design</i>	Adrian Hannon	UL	

P48	<i>In Search of Highly Emissive Donor-Acceptor Structures for Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes</i>	Martha Gulman	TCD	
P49	<i>Design of Coordination Networks using Rod Building Blocks</i>	Daniel J.O’Hearne	UL	
P50	<i>Switching Adsorbent Layered Materials</i>	Shi-Qiang Wang	UL	
P51	<i>Investigation of Steel Serving Utensils on the Irish Market for Migration of Metals using ICPMS</i>	Xinyi Wu	TU Dublin, City Campus	
P52	<i>Development of Novel Anticancer Agents Targeting Glioblastoma Multiforme</i>	Kate Byrne	TU Dublin, City Campus	
P53	<i>A Simple Nanoparticle-Based TiO₂ Memristor Device and the Role of Defect Chemistry in its Operation</i>	Rafaela C de Carvalho	TU Dublin, City Campus	