

# ASIA 2024 MALAYSIA

The 18<sup>th</sup> Conference of the  
Asian Crystallographic Association

**1 – 6 DECEMBER**  
Kuala Lumpur Convention Centre, Malaysia

Crystallography today:  
Beyond the fundamental science

**E-ABSTRACTS BOOK**

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# MS1-1:

# Macromolecular Complexes & Assemblies

Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-013	X-Ray and CryoEM Structures of the Cell Division Protein FtsZ	Hiroyoshi Matsumura
PS-023	Understanding of Sterol Binding with NPC1L1-NTD by V55L Mutation: A Modeling Study	Hyejin Yoon
OR-026	Integrative Structural Biology Approach to Study Structure and Function of Bacterial Flagellar Motor	Anna Roujeinikova
OR-089	Drug-Induced Intersubunit Rotation is a Key Factor for Stop-Codon Read-Through Enhancement	Albert Guskov
OR-092	Structural Basis of the Induction of Synapse Formation by Receptor Protein Tyrosine Phosphatase $\delta$	Shuya Fukai
OR-110	The Structure of the Rat Vitamin B12 Transporter TC and Its Complex with Glutathionylcobalamin	Marcel Bokhove
OR-134	Insights into the Molecular Recognition Mechanism of a Headless Lipid by Natural Killer T Cells	Praveena Thirunavukkarasu
PS-140	Structure of hPRMT1 in Complex with Methylation Cofactor SAH	Sachiko Toma-Fukai
OR-170	Ferritin-Mediated Anticancer Drugs Delivery: Crystallographic, Analytical and Cytotoxicity Studies	Giarita Ferraro
PS-184	Structural Investigation of the Docking Domain Assembly from Trans-AT Polyketide Synthases	Se-Young Son
OR-232	Structural Biology of Viruses and Capsid Assembly	Chun-Jung Chen
PS-258	Molecular Mechanism of Immunoglobulins	Junyu Xiao

OR-299	Unravelling Copper Trafficking in Mitochondria – A Structural Biology Perspective	Megan Maher
PS-303	Crystal Structure of 4-hydroxyphenylacetate-3-monooxygenase from <i>Geobacillus Mahadii</i> Geo-05	Nur Asyikin Che Husain
OR-309	LAG-3 Mediated Regulation of Cellular Immunity	Jan Petersen

# **MS1-II:**

# Protein-Nucleic Acids Interactions

Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-002	New Evidence in Human Innate Immune Signalling: dsDNA Binding by the TIR Domain of the MyD88 Adaptor Protein	Zannati Ferdous Zaoti
PS-047	Sulfolobus Solfataricus SegC Regulates Segrosome Formation and Participates in Archaeal Chromosome Segregation	Min-Guan Lin
PS-056	Crystal Structure of Lyophyllin, the First Ribosome-Inactivating Protein in M35 Superfamily	Liu Chok Mei
PS-058	Insights into Chromosome Segregation in Archaea by SegA- and SegB-DNA Complex Structures and Reveal Segrosome Formation	Cheng-Yi Yen
OR-120	Binding and Structural Studies of the Complexes of Type 1 Ribosome Inactivating Protein from Momordica Balsamina with Uracil and Uridine	Sada Nand Pandey
OR-122	Structural Basis for the Molecular Mechanisms of C-to-U mRNA Editing in Plant Organelles	Ryota Urushihara
PS-163	Structure and Function of DNA-Mimicking Anti-CRISPR Proteins	Euiyoung Bae
OR-168	An Archaeal Transcription Factor EnfR with a Novel 'Eighth Note' Fold Controls Hydrogen Production of a Hyperthermophilic Archaeon Thermococcus Onnurineus NA1	Sun-Shin Cha
OR-251	A PPR Protein-Based FRET Sensor for RNA	Charlie Bond
OR-252	DNA-Protein Recognition by Short Anchoring Elements	Xiao-Dong Su
PS-310	A Novel Cas2 / VapD Sub-Family Protein of Burkholderia Pseudomallei	Chyan Leong Ng

# **MS1-III:**

# Disease-Related Protein Structures



Note: Please click on the title to view abstract.

ID	Title	Author
OR-025	Luteolin as Inhibitor of 3CLpro from SARS-CoV-2 Against COVID-19	Wael Rabeh
OR-080	A Novel Conformation-Specific BAK Antibody Enables Assessment of Non-Activated BAK Levels in Cancer Cells	Michelle Miller
PS-083	5-Aminosalicylic Acid (5-ASA) as an Anti-Inflammatory Treatment in Ulcerative Colitis	Kim Hwayoung
PS-084	Structural and Drug Repurposing Study to Identify Inhibitors of SARS-CoV-2 Main Protease (3CLpro)	Kim Hwayoung
OR-098	New Structure of Full-Length Rat MLKL Reveals Novel Interface for Interdomain Communication	Katherine Davies
OR-137	Molecular Mechanisms of Lipid Antigen Presentation to T Cells in Protective or Aberrant Immunity	Adam Shahine
OR-167	Molecular Insights into Metabolite-Mediated T Cell Immunity	Wael Awad
PS-197	Structural Insights Into tau-ack280 Recognition by Monoclonal Antibody y01	Jaewan Park
PS-227	A Computational Analysis of Lymphocyte Integrin $\alpha 4\beta 1$ and Kidney Integrin $\alpha 8\beta 1$ as Alternative Receptors for the SARS-CoV-2 Spike Protein	Samantha Joei Panday
PS-228	Computational Analysis of SARS-CoV-2 Spike Protein Interactions with RGD-Binding Integrins $\alpha v\beta 6$ , $\alpha v\beta 8$ , and $\alpha IIb\beta 3$	Iustus Maximus Nas
OR-237	Importance of Active Site Residues and Its Substitutions in Plasmodium Pepsin-Like Aspartic Proteases	Satadru Chakraborty

OR-297	Exploring the Molecular Machinery of Cell Death to Discover New Drug Targets	Peter Czabotar
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# **MS1-IV:**

# Membrane Proteins: Structure and Function

Note: Please click on the title to view abstract.

ID	Title	Author
OR-068	Structural Mechanistic Insights into the Function of Phosphatidylethanolamine N-Methyltransferase PmtA Mediating Bacterial Phosphatidylcholine Synthesis	Salma Dienta Salsabila
PS-079	Structural Basis for Membrane Association and Catalysis by Phosphatidylserine Synthase in Escherichia Coli	Eunju Lee
PS-131	Crystal Structure of the Multidrug Efflux Transporter MexB Under Neutral Conditions	Yushi Ueda
OR-194	Antibody-Assisted Cryo-EM Single-Particle Analysis on Intramembrane Metalloprotease RseP from Aquifex Aeolicus	Terukazu Nogi
OR-254	Structural Insight into the Membrane Organization of Red Blood Cells	Ning Gao

# MS1-V: Enzymes and Enzyme Inhibitors: Drug Discovery

Note: Please click on the title to view abstract.

ID	Title	Author
PS-010	Understanding the Structural Basis of Parasite and Host Aminoacyl-tRNA Synthetases Aids in the Design of Potent Inhibitors	Yogavel Manickam
OR-022	Structural Basis of Potent Inhibition of the Cancer-Promoting DNA-Mutating Enzyme APOBEC3A	Geoffrey Jameson
OR-027	Structural and Functional Attributes Among the Leptospiral Outer Surface Multi-Domains Protein	Mohd. Akif
OR-032	Unraveling the Versatility of Polyethylene Glycol on the Regulation of Falcipain 2 Activity	Sampa Biswas
OR-035	A Bacterial Cell-Wall Component Induces Extensive Electrostatic Remodeling and 20,000-Fold Activation in an Antibiotic Discovery Target from Pseudomonas	Kurt Krause
PS-036	Preliminary in Silico Study of Selected Schiff Base Ligands as Potential Japanese Encephalitis Virus Inhibitor	Afiq Azil
OR-037	Structural Analysis and Inhibition of Thymidine Kinase from the Multi-Drug Resistant Strain of Staphylococcus Aureus	Anam Ashraf
OR-094	Structural and Biophysical Properties of Therapeutically Important Proteins Rv1509 and Rv2231A of Mycobacterium Tuberculosis	Nilisha Rastogi
PS-107	X-Ray Structure of $\theta$ -Type Carbonic Anhydrase from Marine Diatom Phaeodactylum Tricornutum	Hiroto Negoro
OR-146	Crystal Structure Analyses of Plasmodium Falciparum 1-Deoxy-D-Xylulose 5-Phosphate Reductoisomerase in Complex with a New Inhibitor	Nobutada Tanaka

OR-162	Crystal Structures of Polymerase Eta-Ligand Complexes for Drug Discovery	Debanu Das
OR-179	Exploiting Cancers Metabolism: A Structural Focus on Malic Enzyme Inhibitors	Ben Krinkel
OR-182	Antibiotics Discovery Based on Structural Information of Toxin-Antitoxin System of Pathogenic Bacteria	Bong-Jin Lee
PS-196	Structural Study of a Putative Aspartic Proteinase from <i>Bacteroides Fragilis</i>	Junghun Kim
OR-214	Structural and Functional Insights into DsbA Substrate Binding Mode Diversity	Taylor Cunliffe
OR-219	Structural Characterization of Class A $\beta$ -Lactamase CESS-1 from <i>Stenotrophomonas Sp.</i> : Insights into Its Substrate Preference	Myeong-Yeon Kim
PS-238	Discovery of a Novel NAMPT Inhibitor for Targeting NAPRT-Deficient EMT-Subtype Cancer Cells and Reducing Chemotherapy-Induced Peripheral Neuropathy	Bu-Gyeong Kang
OR-245	Crystallization and Preliminary X-Ray Crystallographic Analysis of a Promiscuous Paraoxonase from a Locally Isolated Organophosphate-Degrading <i>Bacillus sp. S3wahi</i>	Ameera Azman
PS-257	Crystallization and Preliminary Structural Insights of Thermophilic Carboxylesterase from <i>Anoxybacillus Geothermalis D9</i>	Nurul Fatin Yusrina Ab Rahman
OR-294	Structural Analysis of the ATPase Domain of <i>Mycobacterium Tuberculosis</i> DNA Gyrase in Complex with a Novel Antitubercular Agent	Nei-Li Chan

**MS1-VI:**

# Hot Structures in Biology



Note: Please click on the title to view abstract.

ID	Title	Author
OR-059	Insecticidal Proteins from Ferns Resemble Bacillus Thuringiensis Toxins	Megan Maher
OR-121	Crystal Structure of Mosquito Tyrosylprotein Sulfotransferase	Mariko Kondo
OR-127	Crystal Structure of Arabidopsis Thaliana Sulfotransferase SOT18 Involved in Glucosinolate Biosynthesis	Rio Hirata
PS-129	X-Ray Crystallography of Ferredoxin from Antarctic Green Alga Chlamydomonas Priscuui	Nana Yamamoto
PS-130	Neutron Crystallographic Analysis of Ferredoxin-NADP+ Reductase	Midori Uenaka
OR-181	See the Taste - Structures of Taste Receptors and Their Biological Relevance	Atsuko Yamashita
PS-199	Unveiling Thermostable sPLA2 from Sciscionella Marina: Enhanced Stability and Biotransformation for Industrial Applications	Yeon-Ju Jung
PS-209	Albumin-Based Photosensitizer for Selective Tumor Targeting	So-Yeon Youn
OR-295	Structural Basis of Amyloid Aggregation in Neurodegenerative Diseases	Cong Liu

**MS2-1:**

# Hot Structures in Chemistry

Note: Please click on the title to view abstract.

ID	Title	Author
OR-018	Structure Analysis and Data Discussion of Azo-Leucine Schiff Base Cu(II) Complex	Takashiro Akitsu
PS-045	Co-Crystal of 2-Amino-6-Methyl Pyridine with Diphenylacetic Acid: Synthesis, X-Ray Structure, Quantum Chemical, Hirshfeld Surface Analysis and Antibacterial Activity	Rajni Kant
OR-055	Polynuclear Te-Group 6 (Mo, W)-CO Clusters and Their Oxidized or Coinage Metal-Inserted Products: Syntheses, Structures, and Semiconductivities	Yu-Huei Li
OR-062	Sulfide Containing Silver Nanoclusters Protected by 3-Aminopropanethiolato Rhodium(III) Metalloligands	Zi Lang Goo
OR-105	Breaking Barriers in Single Crystal X-Ray Diffraction: Next Generation Microfocus X-Ray Source & High-Temperature Set Up	Prathapa Siriyara Jagannatha
OR-115	High-Resolution X-Ray Powder Diffraction Reveals Lattice Distortion of Surface and Bulk Regions in Morphology-Controlled Nanocrystals	Bo-Hao Chen
OR-154	Molecular Crystalline Host Systems Based on Indanedione Dimers: Structures and Properties	Yumi Yakiyama
OR-169	Protein Metalation by V-based Drugs: Structural Studies	Antonello Merlino
OR-239	Guest-Regulated Structural Changes of Mechanically Interlocked Polymers	Eunji Lee
OR_250	2D-Polymeric Structure and Hirshfeld Surface Analysis Studies of Dicyanamide-Bridge Complexes of UMCC-6 and UMCC-7	Husni Wahyu Wijaya
OR-278	Adventures in Natural Product Crystallography	Ian Duncan Williams

OR-292	Proton-Electron Coupled Functionalities in Molecular Crystals	Hatsumi Mori
PS-301	A Novel Structure of One-Dimensional Polymeric Nickel(II) Complexes with WO <sub>4</sub> as Bridging Ligands	I Wayan Dasna

# MS2-II: MOFs and Hybrid Materials

Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-033	Crystal Engineering of Dynamic, 2-Periodic MOFs as Hosts for Included Solvents, Gases and Water Vapour	Clive Oliver
PS-065	Structural characterization of Metal-Organic Frameworks (MOFs) Using Non-Ambient In-Situ X-Ray Diffraction	Umesh Tiwari
PS-087	Influence of Temperature on Formation of Metal-Organic Frameworks and Their Application in Sorption of Gases and Water Vapor	Chiranjib Gogoi
OR-090	MOFs Beyond MOFs	Masaki Kawano
PS-091	Modulation of Coordination Network Crystallization Through Magnetic and Thermodynamic Effects	Qiao Jiang
OR-097	Atomic Resolution Structure Analysis Inside a MOF with Adaptable Water Networks	Yuki Wada
OR-104	Tricks to Obtain the Best Structural Information of Challenging MOF/MOC Samples with SC-XRD	Zhenyi Zhang
PS-118	Selective Adsorption of Selenite from Water Using Amorphous Porous Fe-BTC	Asong Byun
PS-119	Cu-Paddlewheel-Based Metal-Organic Polyhedra as Heterogeneous Catalysts for Selective Oxidation	Bogyeong Go
PS-153	Robust In(Imtb)-MOF and Cd(4,5-Imdb)-MOF for Lewis-Acid Assisted Catalysis and Selective Sensing of Picric Acid	Anjali Rajora
OR-190	Colorimetric Decoder Embedded in Metal-Organic Framework Sensor for Optical Identification of Acid Vapors	Jin Yeong Kim

PS-204	Structural Change in the Early Stage of CO <sub>2</sub> Adsorption on Porous Coordination Polymer CID-5	Yoshiki Kubota
OR-205	Up-Down Approach for Expanding the Chemical Space of Metal-Organic Frameworks	Jiyeon Kim
PS-224	Study on the Consecutive Transformation Mechanism in Coordination Polymer Using Neutron Diffraction	Yao Jing
OR-241	Multi-Mode Luminescence Mechanisms and Applications of MOF Systems	Mei Pan
PS-246	Colorimetric Identification of Colorless Acid Vapors using a Metal-Organic Framework-Based Sensor	Hyejin Yoo
OR-264	Exploring the Impact of Structural and Chemical Properties on Photocatalytic Hydrogen Production in Metal-Organic Frameworks	Sareeya Bureekaew
OR-265	Porous Coordination Materials for Electrocatalytic Synthesis of Organonitrogen	Guangqin Li
PS-270	Advancing Defect Engineering in UiO-Type Metal-Organic Frameworks via Solvent-Assisted Ligand Incorporation	Dopil Kim
PS-293	The Bio-MOF Hybrid Complexes of M-BTC-Dextran (M= Gd (III), Mn (II)): Structure and Crystal Growth Studies via Sonochemical Synthesis	Nur Aini
PS-306	Structural Characteristic of a 3D Erbium(III)-Squarate Coordination Polymer Comprising the Hexanuclear [Er <sub>6</sub> (μ <sub>3</sub> -OH) <sub>8</sub> ] Secondary Building Unit	Pacharapon Jearanaiwiwat
PS-307	Crystal Engineering of 3D Layered-Pillared Frameworks of Rare-Earth Based Porous Coordination Polymer	Kanthida Kummoon

PS-308	Crystal Structure of A New One-Dimensional Zinc(II) Coordination Polymer Containing 4,4'-Bipyridine and m-Nitrobenzoate Ligands	Sirinan Thanma
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# MS2-III:

## Solid State Reactions and Dynamics

Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-007	Mechanochemical Preparation of Binary Pharmaceutical Solid Forms: Characterization and Determination of Dissolution Profiles	Juan Manuel Germán-Acacio
OR-016	In Situ Control of Solid State [2+2] Photodimerization of Styrylpyridine by Crystalline-State Photoisomerization	Akiko Sekine
OR-057	Responsive Metal-Organic Frameworks for Structural and Colorimetric Transformation	Jinhee Park
PS-074	Dynamics of Lattice Structure Leading to the Photo-Induced Phase Transition in VO <sub>2</sub> Thin Film	Le Nguyen
OR-148	Efficient Mechanochemical Synthesis of Polyvalent Iodine Salts and Understanding their Reactivities in the Crystalline State	Ipsha Shruti
OR-176	Mechanically Induced Energy Conversion in Polymorphic Single Crystals	Durga Prasad Karothu
OR-240	Solid-state [2+2] Photo-Cycloaddition and Dynamics in Zn(II) Supramolecular Isomers Assembled with Olefin Ligands	In-Hyeok Park

# **MS2-IV:**

# Structure and Properties of Functional Materials

Note: Please click on the title to view abstract.

ID	Title	Author
OR-015	Structure and Phase Transitions in Niobium Doped Na <sub>1/3</sub> La <sub>1/3</sub> Sr <sub>1/3</sub> ZrO <sub>3</sub> Perovskite-Type Sodium-Ion Conductors	Siegbert Schmid
OR-031	Design of High-Performance Defective Graphite-Type Anodes for Sodium-Ion Batteries	Wang Hay Kan
OR-034	Promoting High-Voltage Stability Through Local Lattice Distortion of Halide Solid Electrolytes	Hua Yang
OR-039	Photomechanical Crystals as Light-Activated Organic Soft Robots	Ejaz Ahmed
PS-063	Observation of Solid-Liquid Phase Transition in Organic-Inorganic Hybrid Material Using Simultaneous Measurement of Photoluminescence and X-Ray Total Scattering Data	Seiya Shimono
PS-066	Photocatalysis in Harsh Environments by Using of GaN NWs Grown by PA-MBE	Cosmin Romanitan
OR-069	Controlling the Mechanochromic Luminescence of Organic Crystals Composed of Substituted Benzothiadiazole Derivatives	Suguru Ito
PS-070	In-Situ Observation of Crystal Structure Destruction Process During Heat Treatment in Ni <sup>2+</sup> -Al <sup>3+</sup> Layered Double Hydroxides	Kohei Makishima
PS-072	Rietveld Structural Analysis and Spectroscopic Studies of Pr <sup>3+</sup> Modified Lamellar Type K <sub>2</sub> SrVO <sub>4</sub> Nanophosphors for Luminescent Applications	Neha Lalotra
PS-078	Mechano- and Thermoresponsive Turn-On Luminescence of a Crystalline Bisimidazolyl BINOL Derivative	Honami Murata

PS-103	Solvation-Controlled Photochromism of N-Salicylideneaniline Metal Complex Crystals	Yuko Kishida
PS-123	Hybrid Structure Analysis of Electrocatalysts by Combining X-Ray Diffraction, Absorption, and Scattering	Kiyohiro Adachi
PS-125	Discovery of Novel Non-Perovskite Dual-Ion Conductor	Nozomi Aoki
PS-126	High Proton Conductivity by Donor Doping into Oxides with Intrinsic Oxygen Vacancies	Kensei Umeda
OR-135	Growth of L-Asparagine Monohydrate Organic Single Crystal for Nonlinear Optical Applications: An Experimental and Theoretical Investigation	Jiban Podder
OR-141	Crystal Structure, Polymorphism and Re-Entrant Phase Transition in NaSrPO <sub>4</sub>	Umesh Tiwari
PS-195	Extended Unit Cell Model with Two Vectors for Crystal Structure Analysis of Alloy Nanoparticles	Hiroataka Ashitani
PS-208	Structure Characterization and Physical Properties of New Fe(II) Complexes Chelated by 2-(2-(4-Fluorobenzyl)-2H-Tetrazol-5-yl) Pyridine Ligands	Feng-Hua Ho
PS-211	Dynamic Disorder of Isolated [BO <sub>3</sub> ] Groups in the Ba Fluoride Borates	Nursultan Sagatov
PS-212	Crystal Structures and Thermodynamic Stability of BeCO <sub>3</sub>	Sagatova Dinara
OR-216	Crystal Structure Analysis of Oxygen Absorbed and Released Phases of Layered Oxides YbMn <sub>1-x</sub> Ti <sub>x</sub> O <sub>3+δ</sub>	Hiroki Ishibashi
PS-217	New High-Pressure Phases of Alkali Metal Pyrocarbonates	Maksim Banaev
OR-225	Visualizing Proton Conducting Paths and Revealing Structure-Conductivity Relationship in Some Organic Salts Containing Imidazole and Dicarboxylic Acids	Anucha Koedtruad

OR-244	Electrically Conductive Metal-Organic Framework Thin Films	Sarah Sunah Park
OR-263	Hidden Heterometallic Interaction Emerges from Tb-L3 Resonant Inelastic X-Ray Scattering in Ln–Pt Molecule	Takefumi Yoshida
PS-269	Synthesis, Structure, Antibacterial, and Magnetic Properties Complexes of Ni(4-ampy) <sub>x</sub> (dca) <sub>2</sub> (x= 2 or 4; dca= dicyanamide ion)	Sutandyo Laksamana
PS-273	High-Pressure Synthesis and Electronic Properties of Ilmenite-Type MnGeO <sub>3</sub>	Ippo Aoki
OR-274	Strain-Induced Phase Transformation in Zr-doped HfO <sub>2</sub> Thin Films	Pin-Jiun Wu
PS-279	Polymorphism of an AIEgen Natural Product, HMPQ	Herman Sung
PS-291	All About MyD88: Human IRAK4 Inhibits Spontaneous Filament Formation of Both Human and Bat MyD88-DD	Zannati Ferdous Zaoti

# MS2-V: Crystal Engineering

Note: Please click on the title to view abstract.

ID	Title	Author
OR-017	Design of Multicomponent Piperine Crystals by Crystal Engineering and Structure-Dissolution Correlation	Hidehiro Uekusa
OR-040	Role of Polymorphism in Treating Hair Loss	Sourabh Payal
OR-095	Exploring Solid State Diversity in Chlorpropamide	Anila M Menon
PS-100	Crystal Structure and Dissolution of Acyclovir Multicomponent Crystals	Kaito Matsumoto
PS-101	Crystal Structure and Dissolution Improvement Mechanism of Meloxicam Multicomponent Crystals	Yukihito Akiyama
PS-106	Packing Polymorphism with High ( $Z' = 3$ ) in N-(4-cyanophenyl)-3-Fluorobenzamide	Shubham Som
OR-132	Cocrystallization of Niclosamide to Improve Its Dissolution Property	Il Won Kim
PS-133	Synthesis and Structural Investigation of Coordination Compounds with Quinazoline Derivative Ligands	Kambarali Turgunov
OR-142	Modulation of Stimuli Responsive Dynamic Effects in Crystalline Coordination Polymers: A Crystal Engineering Approach	Bibhuti Bhusan Rath
PS-150	Influence of Glucose Derivatives as Modifiers on Calcium Oxalate Monohydrate Crystallization	Gideon Divinagracia
OR-165	On the Ab Initio Engineering of the Mechanical and Optoelectronic Properties of Molecular Crystals Using Modern Atomistic and Machine Learning Methods	Sharmarke Mohamed
OR-180	Tuning the Properties of Lanreotide via Crystal Engineering	Shuai Wang
OR-187	Photomechanical Effects in Metal-Organic Crystals	Mohammad Hedayetullah Mir



OR-192	Thermal Topochemical Polymerization Reactions: Challenges and Opportunities	Kana M Sureshan
OR-203	Co-Crystals and Salts of Antifolate and Antibacterial Drug-Trimethoprim and Sulfamethazine with Heterocyclic Co Farmers	Sathishkumar Ranganathan
OR-262	Chalcogen Bond: An Emerging Tool in Crystal Engineering	Arun Dhaka
OR-281	To CocrySTALLize or Not? Importance of HeterosynthoN Strength in 11-Azaartemisinin CocrySTALLs with Salicylic and Benzoic Acids	Keyao Li
PS-282	Aluminium Mandelates: Chiral Molecular Rings, Wheels and Dimers	Sam K-S. Lau
PS-284	Molecular Perturbation of Theophylline to 8-Chlorotheophylline: Effect on Polymorphism and CocrySTALL Formation	Chao Zhang
PS-285	Search for Conglomerate Salts to Assist in Challenging Resolutions	Jiawen Li
PS-286	Bulky Chiral Natural Product Acids for Resolution of Challenging Racemic Amines	Cengan Wang
PS-287	Alkaloid: Flavonoid CocrySTALLs: H-Bond Donor-Acceptor Driven CocrySTALLization	Weijian Ye
PS-288	Resolution of Sec-Butylamine Using Copper Mandelate Complexes	Lawrence W-Y. Wong
PS-300	Exploring Substituent Effects in Naphthalene-Derived Salts Towards Crystal Packing	Irene Ling

# MS2-VI:

## Weak Interaction and Supramolecular Chemistry

Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-044	Exploring Proton Tautomeric Pathways to Unveil Distinct Behavior of Polar Polymorphic Forms: A Quantum Crystallographic Approach	Yogita Gupta
OR-048	Versatile Fluorescence on Single Crystals of Non-Stoichiometric Hydrogen-Bonded Organic Frameworks Depending on the Component Fraction and Distribution	Taito Hashimoto
PS-049	Synthesis and Structural Control of Square Planar i-mnt Coordination Complexes Decorated with Cu <sub>4</sub> I <sub>4</sub> Crown Motif	Shunsuke Tanaka
OR-051	Elucidation of Stability of Co-Crystals of Caffeine-Dicarboxylic Acid Complexes by Quantum Crystallography	Kunihisa Sugimoto
OR-053	Constructing Coordination Polymers and Cages from Low-Symmetry and Chiral Ligands	David Turner
PS-054	Polymerization and Depolymerization of Dicyanobenzene-Linked, E-Fe-Cu (E = Te, Se) Clusters: Syntheses, Adsorption / Desorption, and Weak Interactions	Minghuey Shieh
PS-099	Structural Similarity and Chloro-Methyl Exchange Rule for Drug-Drug Multicomponent Crystals of Mefenamic Acid and Tolfenamic Acid	Haruto Ishikawa
PS-113	Delipidation of Human Fatty Acid-Binding Proteins by Protein Refolding	Seina Maekawa
PS-144	Interactions of Carboxylate-Functionalized Hydrogen-Bonded Organic Frameworks with Uranyl Ions in Aqueous System	Jinkyu Park
OR-145	Self-Assemblies of Sulpha-Drug Derived Amides	Jubaraj Bikash Baruah

OR-172	Self-Assembly of Tripeptides into Rigid Supramolecular Materials	Hema Kuntrapakam
OR-215	The Role of Supramolecular Interactions in Recognition of Isostructurality	Petra A Bombicz
PS-283	New Guanidinium 4,4'-Biphenyldisulfonate Framework	Michael H-T. Ho

# MS3-1: Synchrotron and Neutron Applications

Note: Please click on the title to view abstract.

ID	Title	Author
OR-060	Atomic Scale Structure of 2D Atomic Layer Materials, WSe <sub>2</sub> and Graphene, Using SR Micro-Focused X-Ray Beam	Yosuke Ogawa
OR-064	Neutron Diffraction Study of Ice Up to 100 Gpa	Kazuki Komatsu
PS-076	Combined X-Ray Diffraction and Pair Distribution Function Analysis of LaB <sub>6</sub> and CeO <sub>2</sub> Mixtures: Structural Insights Across Varying Ratios	Yu-Chun Chuang
OR-088	Atomic Scale and Electronic Structure Characterization of Amorphous Tantalum Oxide Thin Films via Synchrotron X-Ray Techniques	Loku Singgappulige Rosantha Kumara
PS-096	Evaluation of the Effect of Measurement Time on the Determination of Hydrogen Atom Positions by Single-Crystal Neutron Diffraction	Takashi Ohhara
PS-124	Current Status of Macromolecular Crystallography Beamlines at SPring-8	Naoki Sakai
OR-151	Single-Crystal Neutron Diffraction - Contributions to Quantum and Chemical Crystallography - Models from Crystallography and Their Proper Application	Alison Edwards
PS-185	Crystal and Magnetic Structure of Inorganic-Organic Hybrid (C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> ) <sub>2</sub> M <sub>3</sub> Cl <sub>4</sub> (Me=Cu <sup>2+</sup> , Mn <sup>2+</sup> )	In-Hwan Oh
PS-186	PILATUS4 Hybrid Photon Counting Detectors for Efficient and Fast X-Ray Diffraction	Takeyoshi Taguchi
PS-191	Commission Status Report of Single Crystal X-Ray Diffraction Beamline at TPS	Jey-Jau Lee

PS-202	New Features in Z-Rietveld Version 2.1.2	Takashi Kamiyama
OR-218	Submillisecond in Situ X-Ray Diffraction Measurement System Using Diamond Anvil Cells at Beamline BL10XU/SPring-8	Saori Kawaguchi- Imada
PS-223	Development of Millisecond Time-Resolved Synchrotron Powder Diffraction System Synchronized with Gas Pressure Control	Shogo Kawaguchi
PS-226	SPring-8 BL44XU: Macromolecular Assemblies	Keisuke Sakurai
OR-243	The Design and Current Status of the High-Resolution Neutron Diffractometer at China Spallation Neutron Source	Ping Miao
PS-247	Zero Thermal Expansion in NdBaCo <sub>2</sub> O <sub>5.5+x</sub>	Dong Zhang
PS-248	A New Approach to Teaching the Structure Determination with MX and Cryo-EM	Ruslan Sanishvili
PS-256	ADS-1 and ADS-2: New High-Energy X-Ray Diffraction Beamlines for Advanced Materials Characterisation at the Australian Synchrotron	Josie Auckett
OR-259	Synchrotron X-Ray and Neutron Diffraction Methods for Understanding and Improving the Performance of Energy Materials	Josie Auckett

# MS3-II: XFEL Applications



Note: Please click on the title to view abstract.

<b>ID</b>	<b>Title</b>	<b>Author</b>
PS-061	Serial Femto-Second Crystallography of Simple Inorganics with CCTBX	Kazuki Ota
OR-183	Research Opportunities for Biology at PAL-XFEL	Jaehyun Park
PS-193	Serial Femtosecond Crystallography of Photoswitchable Fluorescent Protein rsGamillus	Eiichi Mizohata
OR-271	Three-Dimensional Molecular Movies of Structural Changes in Proteins Captured by X-Ray Free Electron Lasers	Eriko Nango

# MS3-III: Electron Diffraction and Cryo-EM

Note: Please click on the title to view abstract.

ID	Title	Author
PS-003	Inhibitors Targeting $\alpha$ -Synuclein Fibril's Disordered Region Reduces Pathological Activities in Parkinson's Disease	Cong Liu
PS-004	Different Charged Biopolymers Induce $\alpha$ -Synuclein to Form Fibrils with Distinct Structures	Dan Li
OR-012	Atomic Ionisation Determined by Dynamical Multipole Refinement Against 3D Electron Diffraction Data	Ashwin Suresh
OR-024	Structure Detail Studies by 3D ED	Junliang Sun
OR-052	Capturing Filamentous Protein Complexes of TIR Domains by Using "Small Molecule Glues"	Sulin Li
OR-108	Dynamical Refinement on 3D Electron Diffraction Data of Inorganic and Organic Compounds	Hrushikesh Chintakindi
OR-158	Measuring the Unmeasurable: Getting Structures from Nano-Crystals with the XtaLAB Synergy-ED	Fraser White
PS-161	4-Dimensional Scanning Transmission Electron Microscopy (4D-STEM): An Emerging Technique for Imaging and Structure Determination	Karsten Knorr
OR-171	Charge Density Refinement on 3D Electron Diffraction Data for Organic Crystals	Anil Kumar
OR-233	Decoding the Allosteric Switches of the NADP-Specific Glutamate Dehydrogenases (GDHs)	Arpan Banerjee
OR-255	Comparison of Crystallography and Cryo-EM: Present and Future	Ming-Daw Tsai
OR-260	Tomography Studies of the Dengue Fusion Process	Shee Mei Lok

OR-266	Accurate Simulation of Continuous Precession Electron Diffraction Tomography Based on Golden-Cut Sampling and Its Numerical Properties	Zeyue Zhang
OR-280	B-DNA Crystal Structure Determined by Electron Diffraction	Zhipu Luo

# **MS3-IV:**

# Complementary Methods for Crystallography Beyond Diffraction

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ID	Title	Author
OR-046	Domain Resolved Multiscale Structure Analysis of LaAlO <sub>3</sub> Perovskite	Eiji Nishibori
PS-159	XtaLAB Synergy: Hardware and software in Synergy	Fraser White
OR-188	Rattling of Ag Atoms Found in Low Temperature Phase of Thermoelectric Argpyrodite Ag <sub>8</sub> SnSe <sub>6</sub>	Seiya Takahashi
OR-189	In-Operando Battery Cell and In-Situ Reaction Investigations in Transmission Geometry	Laura Christina Folkers
OR-206	Characterization of sSolvent and Ligand Effects on the Phase Transition Behaviors of Pyridine Based Iron Complexes	I-Jui Hsu
PS-207	Ligand Substituent Effects on a Series of Fe(II) Spin-Crossover Complexes Characterized by X-Ray Powder Diffraction and Absorption Spectroscopy	Jia-Yu Lin
OR-221	Keeping Cool Under Pressure: A Low-Temperature High-Pressure Diamond Anvil Cell for Single-Crystal X-Ray Diffraction	Aston Summers
OR-234	HTK 1500 High-Temperature Chamber, the New Environmental Heater for Non-Ambient X-Ray Diffraction for Crystallographic Investigations of Materials at Very High Temperatures	Benedikt Schrode
OR-242	Pair Distribution Function via Total Scattering Measurement Using "SmartLab" Diffractometer	Yuji Shiramata
OR-261	Self-Assembly of Monodisperse Nanosheets into Columnar Nanofibers	Nobuyoshi Miyamoto

# **MS3-V:**

# Computational Modelling, Databases, and Data Mining

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<b>ID</b>	<b>Title</b>	<b>Author</b>
OR-006	Finding N-Supercells and “1/N” Supercells with Desirable Shape	Yoyo Hinuma
OR-009	In Silico Structural Modelling and Mechanistic Insights of the Alpha Kinase (EIF2AK3) Mediated Translation Regulation	Pavan Kumar Madasu
OR-019	Application of the Powder Diffraction File™ In Materials Characterization	Soorya Kabekkodu
PS-073	Constant pH Molecular Dynamics Simulation on Crystal Structures of ALKBH5-Substrate Complexes to Identify Competitive Inhibitors	Lok Wan Ng
PS-077	AI Sample Centering	Kenji Yoza
OR-093	Experimental Estimation of Statistical Errors in Powder Diffraction Data by Using a Semiconductor Strip Type X-Ray Detector	Takashi Ida
PS-102	Stability Comparison of Perovskite Thin Films by Process Informatics	Ryo Fukasawa
PS-128	Introduction of the Capsules Environment to Support Further Growth of the SBGrid Structural Biology Software Collection	Thomas Nicholson
OR-157	DFT + U Study of the Properties of Tungsten Trioxide, Tungsten Bronzes & Related System	Biplob Deb
OR-178	Application of Molecular Dynamics for Neutron Scattering Experiments	Pablo Galaviz
PS-229	2ClustOrNot2Clust: A Mathematics-Based Screening Method for Viable Protein-Protein Interactions	Iustus Maximus Nas
OR-236	Up-Down Approach: Data-Driven Search Algorithm for Discovery of Synthesizable Metal-Organic Frameworks	Wonyoung Choe



OR-302	Protein Data Bank: The Single Global Archive of 3D Macromolecular Structural Data	Genji Kurisu
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# **MS3-VI:**

# Crystal Growth Techniques

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ID	Title	Author
OR-112	Co-Crystallizing Long Flexible Chain Molecules with Second Generation Chaperons	Martin Adam
OR-160	Diffusion-Controlled Crystallization in a Hydrogel	Sung Ho Yang
OR-166	New Generation Low-Dimensional Nanomaterials for Advanced Water Treatment	Hui Ying Yang
OR-175	Advancing Structural Biology Through AI: Enhancing Macromolecular Crystallography at Nagoya University	Leonard Chavas
PS-200	Control of Bone-like Hydroxyapatite Crystals in a Gelatin Hydrogel	Chae Mi Heo
PS-201	Crystallization of Calcium Carbonate in Hydrogel-Based Cross-Diffusion System	Ki Min Jeong
OR-213	Nanoparticl - Assisted Protein Crystal Growth: Novel Techniques for Optimized Crystallization	Salma Sultana Syed
OR-272	Crystallogenesis in the Age of AI and Cryo-EM	Fasséli Coulibaly
PS-275	The Influence of Low Boron Concentration on the Structural and Optical Quality of B <sub>G</sub> aN Compounds Grown on SiC Substrates	Emil Mihai Pavelescu
PS-289	Absolute Spontaneous Resolution for Transition-Metal(II) and Lanthanoid(III) Complexes	Kazuma Takahara
PS-290	Tailoring the Emission of Self-Assembled InGaAs Quantum Dots by AlGaAs Submonolayer Insertion	Emil Mihai Pavelescu

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