

8th Asia-Pacific NMR Symposium 2019

3 – 6 July 2019

School of Biological Sciences
Nanyang Technological University
60 Nanyang Drive
Singapore 637551

Organised by

8th APNMR Symposium Singapore Committee

~~~~~

## DAY 1: Wednesday, 3 July 2019

|             |                                                                                                                                                                              |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 11:00-14:00 | Registration for Bruker NMR User Pre-Symposium Meeting (School of Biological Sciences Lobby, Bruker's Booth)                                                                 |
| 11:30-13:00 | Lunch for Bruker NMR User Pre-Symposium Meeting (For Meeting Registered Participants only) (School of Biological Sciences Lobby)                                             |
| 13:00-16:30 | Bruker NMR Pre-Symposium User Meeting (ClassRoom 2 – CR2)                                                                                                                    |
| 12:00-20:00 | APNMR 2019 Registration (School of Biological Sciences Lobby)                                                                                                                |
| 17:00-17:02 | Opening Address by <b>Professor Ho Sup Yoon</b> , General Chair (Plenary Lecture Hall - CR1)                                                                                 |
| 17:02-17:10 | Welcome Address by <b>Professor Subra Suresh</b> , President, NTU, Singapore (Plenary Lecture Hall - CR1)                                                                    |
| 17:10-18:00 | Keynote   IAS@NTU Lecture by <b>Prof. Mei Hong</b> , MIT, USA (Plenary Lecture Hall - CR1)<br>“ <b>Nanometer-Distance NMR to Illuminate Protein Structure and Assembly</b> ” |
| 18:00-20:00 | Reception Networking Dinner (L2 Garden or Lobby if Rain)                                                                                                                     |

## DAY 2: Thursday, 4 July 2019

|             |                                                                                                                                                                                                                              |                                             |                                                     |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------|-----------------------------------------------------|
| 8:00-17:00  | Registration (School of Biological Sciences Lobby)                                                                                                                                                                           |                                             |                                                     |
| 9:00-9:40   | Plenary Lecture 1 by <b>Prof. Ichio Shimada</b> , The University of Tokyo, Japan (Plenary Lecture Hall - CR1)<br>“ <b>Function-related Dynamics of Membrane Proteins</b> ”                                                   |                                             |                                                     |
| 9:40-10:20  | Plenary Lecture 2 by <b>Prof. Weontae Lee</b> , Yonsei University, Korea (Plenary Lecture Hall - CR1)<br>“ <b>A New Hybrid Method for Protein Structure and Dynamics: NMR and Serial Femtosecond Crystallography (SFX)</b> ” |                                             |                                                     |
| 10:20-10:40 | Coffee/Tea Break (School of Biological Sciences Lobby)                                                                                                                                                                       |                                             |                                                     |
| Time/Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE & FUNCTION-1                                                                                                                                                              | Venue: ClassRoom 3 (CR3)<br>NMR IN SOLIDS-1 | Venue: ClassRoom 4 (CR4)<br>BIOMOLECULAR DYNAMICS-1 |
| 10:40-11:10 | Norelle Daly<br>(Paper #139)                                                                                                                                                                                                 | John Vincent Hanna<br>(Paper #210)          | Martin Scanlon<br>(Paper #271)                      |
| 11:10-11:40 | Neel Sarovar Bhavesh<br>(Paper #141)                                                                                                                                                                                         | Akira Naito<br>(Paper #125)                 | Dong Long<br>(Paper #148)                           |
| 11:40-12:10 | Bong-Jin Lee<br>(Paper #275)                                                                                                                                                                                                 | Vipin Agarwal<br>(Paper #257)               | Daisuke Kohda<br>(Paper #143)                       |
| 12:10-12:25 | Chunyang Cao<br>(Paper #108)                                                                                                                                                                                                 | Xiangyan Shi<br>(Paper #123)                | Tsyr-Yan Yu<br>(Paper #117)                         |
| 12:25-13:10 | Lunch (School of Biological Sciences Lobby)                                                                                                                                                                                  |                                             |                                                     |

|             |                                                                                                                                              |                                                              |                                                        |
|-------------|----------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------|--------------------------------------------------------|
| 13:10-14:00 | Poster Session #1 (School of Biological Sciences Lobby)                                                                                      |                                                              |                                                        |
| 13:20-13:50 | Sponsor Technical Seminar by<br>See Chung Yip, SCIEX (TR+5)<br>“ Introduction to Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) ” |                                                              |                                                        |
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-2                                                                           | Venue: ClassRoom 3 (CR3)<br>METHODS AND<br>INSTRUMENTATION-1 | Venue: ClassRoom 4 (CR4)<br>BIOMOLECULAR<br>DYNAMICS-2 |
| 14:00-14:30 | Yoshifumi Nishimura<br>(Paper #151)                                                                                                          | Helena Kovacs<br>(Paper #128)                                | Shin-ichi Tate<br>(Paper #153)                         |
| 14:30-15:00 | Konstantin Pervushin<br>(Paper #283)                                                                                                         | Suryaprakash Nagarajao<br>(Paper #120)                       | Yangmee Kim<br>(Paper #133)                            |
| 15:00-15:30 | Yunyu Shi<br>(Paper #149)                                                                                                                    | Kenji Sugase<br>(Paper #131)                                 | Ryo Kitahara<br>(Paper #160)                           |
| 15:30-15:45 | Jie-Rong Huang<br>(Paper #187)                                                                                                               | Konstantin I. Momot<br>(Paper #165)                          | Jae-Hyun Cho<br>(Paper #256)                           |
| 15:45-16:00 |                                                                                                                                              | Fazhan Shi<br>(Paper #150)                                   | Matthias Buck<br>(Paper #104)                          |
| 16:00-16:20 | Coffee/Tea Break (School of Biological Sciences Lobby)                                                                                       |                                                              |                                                        |
| 16:20-16:50 | Shih-Che Sue<br>(Paper #161)                                                                                                                 | Yohei Miyanoiri<br>(Paper #182)                              | Koichi Kato<br>(Paper #269)                            |
| 16:50-17:20 | Congbao Kang<br>(Paper #247)                                                                                                                 | Bikash Baishya<br>(Paper #220)                               | Joon-Hwa Lee<br>(Paper #162)                           |
| 17:20-17:35 | Yunhuang Yang<br>(Paper #112)                                                                                                                | Takanori Kigawa<br>(Paper #245)                              | Masatsune Kainosho<br>(Paper #188)                     |
| 17:35-17:50 | Hidehito Tochio<br>(Paper #233)                                                                                                              |                                                              |                                                        |
| 17:50-18:00 | Gather for Banquet Dinner (School of Biological Sciences Lobby)                                                                              |                                                              |                                                        |
| 18:00-21:00 | Conference Photography & Banquet Dinner @ Raffles Marina Country Club                                                                        |                                                              |                                                        |

### DAY 3: Friday, 5 July 2019

|             |                                                                                                                                                                                                                                           |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 8:00-17:00  | Registration (School of Biological Sciences Lobby)                                                                                                                                                                                        |
| 9:00-9:40   | Plenary Lecture 3 by<br><b>Prof. Joel Mackay</b> , The University of Sydney, Australia (Plenary Lecture Hall - CR1)<br><b>“ RaPID Peptide Library Screening for the Discovery of Selective and High Affinity Bromodomain Inhibitors ”</b> |
| 9:40-10:20  | Plenary Lecture 4 by<br><b>Prof. P.K. Madhu</b> , Tata Institute of Fundamental Research, India (Plenary Lecture Hall - CR1)<br><b>“ Recoupling schemes in solid-state NMR in a Different Light ”</b>                                     |
| 10:20-10:40 | Coffee/Tea Break (School of Biological Sciences Lobby)                                                                                                                                                                                    |

|             |                                                                                                                                                     |                                                                             |                                                                        |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------|------------------------------------------------------------------------|
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-3                                                                                  | Venue: ClassRoom 3 (CR3)<br>NMR IN SOLIDS-2/<br>MATERIALS AND<br>INORGANICS | Venue: ClassRoom 4 (CR4)<br>BIOMOLECULAR<br>DYNAMICS-3                 |
| 10:40-11:10 | Mitsuhiko Ikura<br>(Paper #176)                                                                                                                     | Toshimichi Fujiwara<br>(Paper #146)                                         | Koh Takeuchi<br>(Paper #216)                                           |
| 11:10-11:40 | Vanessa Kay Morris (Paper<br>#223)                                                                                                                  | Sebastian Wegner<br>(Paper #284)                                            | Zhou Gong<br>(Paper #180)                                              |
| 11:40-12:10 | Ke Ruan<br>(Paper #186)                                                                                                                             | Xueqian Kong<br>(Paper #167)                                                | Takumi Ueda<br>(Paper #168)                                            |
| 12:10-12:25 | Keisuke Kamba<br>(Paper #190)                                                                                                                       | Luke Austin O'Dell<br>(Paper #130)                                          | Ewen Lescop<br>(Paper #241)                                            |
| 12:25-13:10 | Lunch (School of Biological Sciences Lobby)                                                                                                         |                                                                             |                                                                        |
| 12:25-14:00 | APNMR Council Meeting for Council Members (Meeting Room 1, Level 1, General Office, SBS)                                                            |                                                                             |                                                                        |
| 13:10-14:00 | Poster Session #2 (School of Biological Sciences Lobby)                                                                                             |                                                                             |                                                                        |
| 13:20-13:50 | Sponsor Technical Seminar by<br>Frint Li, NanoTemper/QIAGEN (TR+5)<br>“ <b>Biomolecular Interaction Analytics using Microscale Thermophoresis</b> ” |                                                                             |                                                                        |
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-4                                                                                  | Venue: ClassRoom 3 (CR3)<br>METABOLOMICS-1                                  | Venue: ClassRoom 4 (CR4)<br>METHODS AND<br>INSTRUMENTATION-2/<br>OTHER |
| 14:00-14:30 | Masato Katahira<br>(Paper #198)                                                                                                                     | Jun Kikuchi<br>(Paper #163)                                                 | Ago Samoson<br>(Paper #281)                                            |
| 14:30-15:00 | Jeong-Yong Suh<br>(Paper #147)                                                                                                                      | Manfred Spraul<br>(Paper #286)                                              | Keunhong Jeong<br>(Paper #183)                                         |
| 15:00-15:30 | Daniel Mathieu<br>(Paper #287)                                                                                                                      | Caroline Rae<br>(Paper #288)                                                | Yun-Wei Chiang<br>(Paper #154)                                         |
| 15:30-15:45 | Xun-Cheng Su<br>(Paper #157)                                                                                                                        | Yulan Wang<br>(Paper #116)                                                  | Ming Wei Chen<br>(Paper #289)                                          |
| 15:45-16:00 |                                                                                                                                                     |                                                                             | Heelim Chae<br>(Paper #263)                                            |
| 16:00-16:20 | Coffee/Tea Break (School of Biological Sciences Lobby)                                                                                              |                                                                             |                                                                        |
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-5                                                                                  | Venue: ClassRoom 3 (CR3)<br>METABOLOMICS –2 / MNR<br>IN SOLIDS-3            | Venue: ClassRoom 4 (CR4)<br>QUANTITATIVE MRS/MRI                       |
| 16:20-16:50 | Lifeng Pan<br>(Paper #177)                                                                                                                          | Neeraj Sinha<br>(Paper #277)                                                | S. Sendhil Velan<br>(Paper #109)                                       |
| 16:50-17:20 | Anirban Bhunia<br>(Paper #144)                                                                                                                      | Shenlin Wang<br>(Paper #292)                                                | Dennis Hwang<br>(Paper #204)                                           |

|             |                               |                            |                                 |
|-------------|-------------------------------|----------------------------|---------------------------------|
| 17:20-17:35 | Tomohide Saio<br>(Paper #250) | Chi-Jen Lo<br>(Paper #194) | Chaejoon Cheong<br>(Paper #260) |
| 17:35-17:50 |                               |                            |                                 |

## DAY 4: Saturday, 6 July 2019

|             |                                                                                                                                                                                    |                                                                                          |                                                                                                                     |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|
| 8:00-11:00  | Registration (School of Biological Sciences Lobby)                                                                                                                                 |                                                                                          |                                                                                                                     |
| 9:00-9:40   | Plenary Lecture 5 by<br><b>Prof. Chun Tang</b> , Chinese Academy of Sciences, China (Plenary Lecture Hall - CR1)<br>“ <b>Modify the Modifier, a Convoluted Tale of Ubiquitin</b> ” |                                                                                          |                                                                                                                     |
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-6                                                                                                                 | Venue: ClassRoom 3 (CR3)<br>METABOLOMICS –3                                              | Venue: ClassRoom 4 (CR4)<br>NATURE PRODUCT                                                                          |
| 9:50-10:20  | Mandar V Deshmukh<br>(Paper #248)                                                                                                                                                  | Oliver A.H. Jones<br>(Paper #282)                                                        | Kaifeng Hu<br>(Paper #145)                                                                                          |
| 10:20-10:40 | Coffee/Tea Break (School of Biological Sciences Lobby)                                                                                                                             |                                                                                          |                                                                                                                     |
| Time\Venue  | Venue: ClassRoom 2 (CR2)<br>BIOMOLECULAR STRUCTURE<br>& FUNCTION-7                                                                                                                 | Venue: ClassRoom 3 (CR3)<br>METHODS AND<br>INSTRUMENTATION-3/<br>BIOMOLECULAR DYNAMICS-4 | Venue: ClassRoom 4 (CR4)<br>MOLECULES IN MEDICINE/<br>BIOMOLECULAR<br>STRUCTURE & FUNCTION-<br>8/COMPUTATION IN NMR |
| 10:40-11:10 | Teppei Ikeya<br>(Paper #270)                                                                                                                                                       | Bjoern Heitman<br>(Paper #285)                                                           | Shang-Te Danny Hsu<br>(Paper #138)                                                                                  |
| 11:10-11:40 | Junxia Lu<br>(Paper #118)                                                                                                                                                          | Pramodh Vallurupalli<br>(Paper #279)                                                     | K. V. R. Chary<br>(Paper #290)                                                                                      |
| 11:40-12:10 | Noritaka Nishida<br>(Paper #252)                                                                                                                                                   | Ramakrishna V. Hosur<br>(Paper #280)                                                     | Chojiro Kojima<br>(Paper #291)                                                                                      |
| 12:10-12:25 | Iktae Kim<br>(Paper #208)                                                                                                                                                          | So Young An<br>(Paper #179)                                                              | Shunji Yamada<br>(Paper 218)                                                                                        |
| 12:35-13:00 | Award / Closing (Plenary Lecture Hall - CR1)                                                                                                                                       |                                                                                          |                                                                                                                     |
| 13:00-14:00 | Lunch (School of Biological Sciences Lobby)                                                                                                                                        |                                                                                          |                                                                                                                     |

Wednesday, 3 July 2019

### BRUKER NMR PRE-SYMPOSIUM USER MEETING

Chair: **Bruker**

|             |                                                                                                                                     |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------|
| 11:00-14:00 | Registration for Bruker NMR User Pre-Symposium Meeting<br>(School of Biological Sciences Lobby, Bruker's Booth)                     |
| 11:30-13:00 | Lunch for Bruker NMR User Pre-Symposium Meeting<br>(For Meeting Registered Participants only) (School of Biological Sciences Lobby) |
| 13:00-16:30 | Bruker NMR Pre-Symposium User Meeting (ClassRoom 2 – CR2)                                                                           |

### SYMPOSIUM OPENING/ KEYNOTE | IAS@NTU LECTURE

Chair: **Prof Ho Sup Yoon**

|             |                                                                                                                                                                                   |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 12:00-20:00 | Registration (School of Biological Sciences Lobby)                                                                                                                                |
| 17:00-17:02 | Opening Address by <b>Professor Ho Sup Yoon</b> , General Chair<br>(Plenary Lecture Hall, CR1)                                                                                    |
| 17:02-17:10 | Welcome Address by <b>Professor Subra Suresh</b> , President, NTU, Singapore<br>(Plenary Lecture Hall, CR1)                                                                       |
| 17:10-18:00 | <b>Keynote   IAS@NTU Lecture</b><br><i>“ Nanometer-Distance NMR to Illuminate Protein Structure and Assembly ”</i><br>Professor Mei Hong, MIT, USA<br>(Plenary Lecture Hall, CR1) |
| 18:00-20:00 | <b>Reception Networking Dinner (L2 Garden or SBS Lobby if rain)</b>                                                                                                               |

Thursday, 4 July 2019

Venue: Plenary Lecture Hall (CR1)

## PLENARY LECTURES-1/2

Chair: **Prof Daiwen Yang**

|             |                                                                                                                                                                                               |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:00-9:40   | <b><i>Plenary Talk 1: “ Function-related Dynamics of Membrane Proteins ”</i></b><br>Professor Ichio Shimada, The University of Tokyo, Japan                                                   |
| 9:40-10:20  | <b><i>Plenary Talk 2: “ A New Hybrid Method for Protein Structure and Dynamics: NMR and Serial Femtosecond Crystallography (SFX) ”</i></b><br>Professor Weontae Lee, Yonsei University, Korea |
| 10:20-10:40 | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                                      |

Venue: Classroom 2 (CR2)

## BIOMOLECULAR STRUCTURE & FUNCTION-1

Chair/Co-Chair: **Norelle Daly / Neel Sarovar Bhavesh**

|                                  |                                                                                                                                                                                                      |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 139</b> | <b><i>Structure/function relationships of granulin peptides</i></b><br>Norelle Daly, James Cook University, Australia                                                                                |
| 11:10-11:40<br><b>Paper# 141</b> | <b><i>Is there a code for single-stranded nucleic acid recognition by RNA Recognition Motifs?</i></b><br>Neel Sarovar Bhavesh, International Centre for Genetic Engineering and Biotechnology, India |
| 11:40-12:10<br><b>Paper# 275</b> | <b><i>Structural study on toxin-antitoxin systems in Pathogenic Bacteria</i></b><br>Bong-Jin Lee, Seoul National University, Korea                                                                   |
| 12:10-12:25<br><b>Paper# 108</b> | <b><i>Mechanistic Studies on Human APOBEC3 Family Members Catalyzed Deamination of Cytidines in DNA by Nuclear Magnetic Resonance</i></b><br>Chunyang Cao, Chinese Academy of Sciences, China        |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                                          |
| 13:10-14:00                      | Poster Session #1 (School of Biological Sciences Lobby)                                                                                                                                              |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b>“ Introduction to Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) ”</b><br>by <b>See Chung Yip</b> , SCIEX                           |

Venue: Classroom 2 (CR2)

## BIOMOLECULAR STRUCTURE & FUNCTION-2

Chair/Co-Chair: **Konstantin Pervushin / Surajit Bhattacharyya**

|                                  |                                                                                                                                                                                        |
|----------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 151</b> | <b><i>Intrinsically Disordered Tails in Chromatin-related Proteins</i></b><br>Yoshifumi Nishimura, Yokohama City University, Japan                                                     |
| 14:30-15:00<br><b>Paper# 283</b> | <b><i>Molecular mechanism of neuroprotective function of a ubiquitous prostaglandin synthase</i></b><br>Konstantin Pervushin, Nanyang Technological University, Singapore              |
| 15:00-15:30<br><b>Paper# 149</b> | <b><i>Mitosis-specific acetylation tunes Ran effector binding for chromosome segregation</i></b><br>Yunyu Shi, University of science and technology of China, China                    |
| 15:30-16:00<br><b>Paper# 187</b> | <b><i>Intrinsically disordered regions of proteins mediate their liquid-liquid phase separation</i></b><br>Jie-rong Huang, National Yang-Ming University, Taiwan                       |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                               |
| 16:20-16:50<br><b>Paper# 161</b> | <b><i>NMR Study of Chemokine Oligomerization Mechanism</i></b><br>Shih-Che Sue, National Tsing Hua University, Taiwan                                                                  |
| 16:50-17:20<br><b>Paper# 247</b> | <b><i>Structural investigation of Zika virus protease and its insight into structure-based drug design</i></b><br>Congbao Kang, Agency for Science, Technology and Research, Singapore |
| 17:20-17:35<br><b>Paper# 112</b> | <b><i>Structural and functional study on the C-terminal repressive domain of human TGIF1</i></b><br>Yunhuang Yang, Wuhan Institute of Physics and Mathematics, China                   |
| 17:35-17:50<br><b>Paper# 233</b> | <b><i>Autosuppression mechanism of the innate immune adaptor protein MyD88 revealed by NMR and High-speed AFM</i></b><br>Hidehito Tochio, Kyoto University, Japan                      |
| 17:50-18:00                      | Gather for Banquet Dinner (School of Biological Sciences Lobby)                                                                                                                        |
| 18:00-21:00                      | Conference Photography & Banquet Dinner @ Raffles Marina Country Club                                                                                                                  |

Venue: Classroom 3 (CR3)

## NMR IN SOLIDS -1

Chair/Co-Chair: **Akira Naito / Vipin Agarwal**

|                                  |                                                                                                                                                                                                                              |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 210</b> | <b><i>A NMR Crystallographic Approach to an Accurate Description of the Disordered Mullite System</i></b><br>John Vincent Hanna, University of Warwick, United Kingdom                                                       |
| 11:10-11:40<br><b>Paper# 125</b> | <b><i>Photointermediates and Photoreaction Cycles of Retinal-Binding Photoreceptor Proteins as Revealed by In Situ Photoirradiation Solid-State NMR Spectroscopy</i></b><br>Akira Naito, Yokohama National University, Japan |
| 11:40-12:10<br><b>Paper# 257</b> | <b><i>Novel Proton-Proton Recoupling Approaches in Fully Protonated solids at very Fast Magic Angle Spinning</i></b><br>Vipin Agarwal, Tata Institute of Fundamental Research, India                                         |
| 12:10-12:25<br><b>Paper# 123</b> | <b><i>Structure and Dynamics of Nucleosomes Investigated by Solid-State NMR</i></b><br>Xiangyan Shi, Nanyang Technological University, Singapore                                                                             |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                                                                  |
| 13:10-14:00                      | Poster Session #1 (School of Biological Sciences Lobby)                                                                                                                                                                      |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b>“ Introduction to Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) ”</b><br>by <b>See Chung Yip</b> , SCIEX                                                   |

Venue: Classroom 3 (CR3)

## METHODS AND INSTRUMENTATION-1

Chair/Co-Chair: **Suryaprakash Nagarajaro / Takanori Kigawa**

|                                  |                                                                                                                                                                                   |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 128</b> | <b><i>Biomolecular interactions monitored by <math>^{19}\text{F}</math> NMR</i></b><br>Helena Kovacs, Bruker BioSpin, Switzerland                                                 |
| 14:30-15:00<br><b>Paper# 120</b> | <b><i>NMR Methodologies and Water Compatible Weak Chiral Aligning Media for Enantiomeric Discrimination</i></b><br>Suryaprakash Nagarajaro, Indian Institute of Science, India    |
| 15:00-15:30<br><b>Paper# 131</b> | <b><i>In situ Monitoring of Amyloid Fibril Formation Processes Using Rheo-NMR</i></b><br>Kenji Sugase, Kyoto University, Japan                                                    |
| 15:30-15:45<br><b>Paper# 165</b> | <b><i>Assessment of Mammographic Density and Breast Tissue Composition by Single-sided Portable NM</i></b><br>Konstantin I. Momot, Queensland University of Technology, Australia |
| 15:45-16:00<br><b>Paper# 150</b> | <b><i>Magnetic Resonance Spectroscopy of A Single Molecule</i></b><br>Fazhan Shi, University of Science and Technology of China, China                                            |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                          |
| 16:20-16:50<br><b>Paper# 182</b> | <b><i>Transverse relaxation optimized isotope labelling for studying structural dynamics of larger proteins</i></b><br>Yohei Miyanoiri, Osaka University, Japan                   |
| 16:50-17:20<br><b>Paper# 220</b> | <b><i>Improved resolution of metabolite peaks in 2D NMR spectra of bio-fluids</i></b><br>Bikash Baishya, Centre of Biomedical Research, India                                     |
| 17:20-17:50<br><b>Paper# 245</b> | <b><i>Selective isotope labelling combined with information science</i></b><br>Takanori Kigawa, Rikagaku Kenkyūjo (RIKEN), Japan                                                  |
| 17:50-18:00                      | Gather for Banquet Dinner (School of Biological Sciences Lobby)                                                                                                                   |
| 18:00-21:00                      | Conference Photography & Banquet Dinner @ Raffles Marina Country Club                                                                                                             |

Venue: Classroom 4 (CR4)

## BIOMOLECULAR DYNAMICS-1

Chair/Co-Chair: **Martin Scanlon / Tsyr-Yan Yu**

|                                  |                                                                                                                                                                            |
|----------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 271</b> | <b><i>Visualising “invisible” states of proteins to support structure-based drug design</i></b><br>Martin Scanlon, Monash University, Australia                            |
| 11:10-11:40<br><b>Paper# 148</b> | <b><i>Probing Slow Motions in Active and Inactive Ras by Relaxation-Based NMR Spectroscopy</i></b><br>Dong Long, University of Science and Technology of China, China      |
| 11:40-12:10<br><b>Paper# 143</b> | <b><i>The lantibiotic nukacin ISK-1 exists in an equilibrium between active and inactive lipid-II binding states</i></b><br>Daisuke Kohda, Kyushu University, Japan        |
| 12:10-12:25<br><b>Paper# 117</b> | <b><i>A combinatorial approach to study lipid composition dependent membrane protein functions</i></b><br>Tsyr-Yan Yu, Academia Sinica, Taiwan                             |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                |
| 13:10-14:00                      | Poster Session #1 (School of Biological Sciences Lobby)                                                                                                                    |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b>“ Introduction to Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS) ”</b><br>by <b>See Chung Yip</b> , SCIEX |

Venue: Classroom 4 (CR4)

## BIOMOLECULAR DYNAMICS-2

Chair: Maili Liu

|                                  |                                                                                                                                                                                                                                |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 153</b> | <b><i>Multiple-phosphorylation in the intrinsically disordered region (IDR) of chromatin remodeler FACT tunes its remodeling activity through conformational dynamics</i></b><br>Shin-ichi Tate, Hiroshima University, Japan   |
| 14:30-15:00<br><b>Paper# 133</b> | <b><i>Thermostabilities, Structures and Dynamics of Proteins from Thermophilic, Mesophilic, and Psychrophilic Bacteria for Thermal Adaptation</i></b><br>Yangmee Kim, Konkuk University, Korea                                 |
| 15:00-15:30<br><b>Paper# 160</b> | <b><i>High-pressure NMR spectroscopy as a tool for studying protein dynamics</i></b><br>Ryo Kitahara, Ritsumeikan University, Japan                                                                                            |
| 15:30-15:45<br><b>Paper# 256</b> | <b><i>Structural and dynamic mechanisms whereby a pandemic influenza A virus antagonizes host antiviral immune responses</i></b><br>Jae-Hyun Cho, Texas A&M University, USA                                                    |
| 15:45-16:00<br><b>Paper# 104</b> | <b><i>Dynamic Protein Complexes : A Perspective from NMR studies and from Molecular Dynamics Simulations for Structure Determination</i></b><br>Matthias Buck, Case Western Reserve University, Germany                        |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                                                                       |
| 16:20-16:50<br><b>Paper# 269</b> | <b><i>NMR characterization of dynamic conformations and interactions of functional oligosaccharides and antibody glycoproteins</i></b><br>Koichi Kato, National Institutes of Natural Sciences & Nagoya City University, Japan |
| 16:50-17:20<br><b>Paper# 162</b> | <b><i>Base-pair opening dynamics study of nucleic acids: Implications for their biological functions</i></b><br>Joon-Hwa Lee, Gyeongsang National University, Korea                                                            |
| 17:20-17:50<br><b>Paper# 188</b> | <b><i>Perspectives on the Aromatic Ring Flipping Dynamics in Proteins</i></b><br>Masatsune Kainosho, Tokyo Metropolitan University, Japan                                                                                      |
| 17:50-18:00                      | Gather for Banquet Dinner (School of Biological Sciences Lobby)                                                                                                                                                                |
| 18:00-21:00                      | Conference Photography & Banquet Dinner @ Raffles Marina Country Club                                                                                                                                                          |

**Friday, 5 July 2019**

Venue: Plenary Lecture Hall (CR1)

### PLENARY LECTURES-3/4

Chair: **Surajit Bhattacharyya**

|             |                                                                                                                                                                                                         |
|-------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:00-9:40   | <b><i>Plenary Talk 3: “ RaPID peptide library screening for the discovery of selective and high affinity bromodomain inhibitors ”</i></b><br>Professor Joel Mackay, The University of Sydney, Australia |
| 9:40-10:20  | <b><i>Plenary Talk 4: “ Recoupling schemes in solid-state NMR in a different light ”</i></b><br>Professor P.K. Madhu, Tata Institute of Fundamental Research, India                                     |
| 10:20-10:40 | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                                                |

Venue: Classroom 2 (CR2)

### BIOMOLECULAR STRUCTURE & FUNCTION-3

Chair/Co-Chair: **Mitsuhiko Ikura / Ke Ruan**

|                                  |                                                                                                                                                                                                    |
|----------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 176</b> | <b><i>Targeting K-RAS4B on Biological Membranes</i></b><br>Mitsuhiko Ikura, University Health Network, University of Toronto, Canada                                                               |
| 11:10-11:40<br><b>Paper# 223</b> | <b><i>Redox-regulated amyloid fibril formation of the tumour suppressor p16</i></b><br>Vanessa Kay Morris, University of Canterbury, New Zealand                                                   |
| 11:40-12:10<br><b>Paper# 186</b> | <b><i>Conformational Selection of Ligand Recognition by PHF20L1 Tudor Domain</i></b><br>Ke Ruan, University of Science and Technology of China, China                                              |
| 12:10-12:25<br><b>Paper# 190</b> | <b><i>An insight into the target search and HIV Vif-dependent inactivation of APOBEC3F and APOBEC3G elucidated by tracking the deamination events</i></b><br>Keisuke Kamba, Kyoto University Japan |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                                        |
| 12:25-14:00                      | APNMR Council Meeting for Council Members<br>(Meeting Room 1, Level 1, General Office, SBS)                                                                                                        |
| 13:10-14:00                      | Poster Session #2 (School of Biological Sciences Lobby)                                                                                                                                            |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b><i>“ Biomolecular Interaction Analytics using Microscale Thermophoresis ”</i></b><br>by Frint Li, NanoTemper/Research Biolabs                |

Venue: Classroom 2 (CR2)

## BIOMOLECULAR STRUCTURE & FUNCTION-4/5

Chair/Co-Chair: Anh Tuan Phan / Xun-Cheng Su

|                                  |                                                                                                                                                                                       |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 198</b> | <b><i>Unique Quadruplex Structure and Anti-disease Activity of RNA Aptamer, and In-cell NMR of Nucleic Acids</i></b><br>Masato Katahira, Kyoto University, Japan                      |
| 14:30-15:00<br><b>Paper# 147</b> | <b><i>Structure and peptidoglycan interaction of the cell wall binding domain of bacteriophage PBC5 endolysin</i></b><br>Jeong-Yong Suh, Seoul National University, Korea             |
| 15:00-15:30<br><b>Paper# 287</b> | <b><i>Verifying Higher Order Structure of Biologics using nuclear magnetic resonance</i></b><br>Daniel Mathieu, Bruker Rheinstetten, Germany                                          |
| 15:30-16:00<br><b>Paper# 157</b> | <b><i>Structural determination of low-abundance enzyme intermediate complex under real-time conditions using paramagnetic labelling</i></b><br>Xun-Cheng Su, Nankai University, China |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                              |
| 16:20-16:50<br><b>Paper# 177</b> | <b><i>Structural insights into the dual functions of NDP52 and TAX1BP1 in selective autophagy</i></b><br>Lifeng Pan, Chinese Academy of Sciences, China                               |
| 16:50-17:20<br><b>Paper# 144</b> | <b><i>Structural and Mechanistic Studies of Amyloids and Model Membranes</i></b><br>Anirban Bhunia, Bose Institute, India                                                             |
| 17:20-17:50<br><b>Paper# 250</b> | <b><i>Structural and kinetic basis for functional modulation of a molecular chaperone</i></b><br>Tomohide Saio, Hokkaido University, Japan                                            |

Venue: Classroom 3 (CR3)

## NMR IN SOLIDS-2/ MATERIALS AND INORGANICS

Chair/Co-Chair: Toshimichi Fujiwara / Xueqian Kong

|                                  |                                                                                                                                                                                                            |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 146</b> | <b><i>Heteronuclear Spin Correlated Components Induced by High-Field Dynamic Nuclear Polarization for Magic-Angle-Spinning Solid-State NMR at 30 K</i></b><br>Toshimichi Fujiwara, Osaka University, Japan |
| 11:10-11:40<br><b>Paper# 284</b> | <b><i>Sensitivity &amp; Productivity Enhancement in Solid State NMR experiments – New Hardware for Accessing the Inaccessible</i></b><br>Sebastian Wegner, Bruker Rheinstetten, Germany                    |
| 11:40-12:10<br><b>Paper# 167</b> | <b><i>Ligands on Nanocrystals: From Molecular Picture to Macroscopic Solubility</i></b><br>Xueqian Kong, Zhejiang University, China                                                                        |
| 12:10-12:25<br><b>Paper# 130</b> | <b><i>New NMR methods for probing interactions and structure in ionic liquids</i></b><br>Luke Austin O'Dell, Deakin University, Australia                                                                  |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                                                |
| 12:25-14:00                      | APNMR Council Meeting for Council Members<br>(Meeting Room 1, Level 1, General Office, SBS)                                                                                                                |
| 13:10-14:00                      | Poster Session #2 (School of Biological Sciences Lobby)                                                                                                                                                    |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b><i>“ Biomolecular Interaction Analytics using Microscale Thermophoresis ”</i></b><br>by Frint Li, NanoTemper/Research Biolabs                        |

Venue: Classroom 3 (CR3)

## METABOLOMICS-1

Chair/Co-Chair: Yulan Wang / Jun Kikuchi

|                                  |                                                                                                                                                                                                        |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 163</b> | <b><i>Data science approach of low- and high-field NMR data from environmental complexities</i></b><br>Jun Kikuchi, Rikagaku Kenkyūjo (RIKEN), Japan                                                   |
| 14:30-15:00<br><b>Paper# 286</b> | <b><i>NMR Based Tools for Clinical Metabolomics</i></b><br>Manfred Spraul, Bruker Rheinstetten, Germany                                                                                                |
| 15:00-15:30<br><b>Paper# 288</b> | <b><i>Brain bioenergetics and magnetic resonance spectroscopy; a systems biochemistry approach</i></b><br>Caroline Rae, Neuroscience Research Australia & The University of New South Wales, Australia |
| 15:30-16:00<br><b>Paper# 116</b> | <b><i>Metabolomics-A great tool for generating hypothesis</i></b><br>Yulan Wang, Nanyang Technological University, Singapore                                                                           |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                                               |

## METABOLOMICS –2 / NMR IN SOLIDS-3

Chair: Congbao Kang

|                                  |                                                                                                                                                                                    |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 16:20-16:50<br><b>Paper# 277</b> | <b><i>Insight into the heterogeneous biology of Acute Respiratory Distress Syndrome (ARDS) by NMR based metabolomics</i></b><br>Neeraj Sinha, Centre of Biomedical Research, India |
| 16:50-17:20<br><b>Paper# 292</b> | <b><i>The Mechanism of Antimicrobial Peptides Characterized by Whole-cell Solid-state NMR</i></b><br>Shenlin Wang, Peking University, China                                        |
| 17:20-17:35<br><b>Paper# 194</b> | <b><i>Metabolic Signature Discovery for Sarcopenia in Elderly Taiwanese</i></b><br>Chi-Jen Lo, Chang Gung University, China                                                        |

Venue: Classroom 4 (CR4)

### BIOMOLECULAR DYNAMICS-3

Chair: Ping-Chiang Lyu

|                                  |                                                                                                                                                                                                                                       |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 216</b> | <b><i>Conformational equilibrium defines variable transcriptional repression of a multidrug binding transcriptional repressor, QacR</i></b><br>Koh Takeuchi, National Institute for Advanced Industrial Science and Technology, Japan |
| 11:10-11:40<br><b>Paper# 180</b> | <b><i>Using Solvent Paramagnetic Relaxation Enhancement to Visualize Biomolecular Structure and Dynamics</i></b><br>Zhou Gong, Chinese Academy of Sciences, China                                                                     |
| 11:40-12:10<br><b>Paper# 168</b> | <b><i>Identification of conformational equilibrium that determines the conductance of P2X4 receptor</i></b><br>Takumi Ueda, The University of Tokyo, Japan                                                                            |
| 12:10-12:25<br><b>Paper# 241</b> | <b><i>A well-balanced preexisting equilibrium governs maximal electron flux efficiency of a multidomain diflavin reductase</i></b><br>Ewen Lescop, Institut de Chimie des Substances Naturelles, France                               |
| 12:25-13:10                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                                                                           |
| 12:25-14:00                      | APNMR Council Meeting for Council Members<br>(Meeting Room 1, Level 1, General Office, SBS)                                                                                                                                           |
| 13:10-14:00                      | Poster Session #2 (School of Biological Sciences Lobby)                                                                                                                                                                               |
| 13:20-13:50                      | Sponsor Technical Seminar (Tutorial Room, TR+5)<br><b><i>“ Biomolecular Interaction Analytics using Microscale Thermophoresis ”</i></b><br>by Frint Li, NanoTemper/Research Biolabs                                                   |

Venue: Classroom 4 (CR4)

## METHODS AND INSTRUMENTATION-2/ OTHER

Chair/Co-Chair: Yun-Wei Chiang / Keunhong Jeong

|                                  |                                                                                                                                                                                |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 14:00-14:30<br><b>Paper# 281</b> | <b><i>H-MAS and other new NMR technologies</i></b><br>Ago Samoson, Tallinn University of Technology, Estonia                                                                   |
| 14:30-15:00<br><b>Paper# 183</b> | <b><i>SQUID-based ultralow field MRI of hyperpolarized material by using SABRE</i></b><br>Keunhong Jeong, Korea Military Academy, Korea                                        |
| 15:00-15:30<br><b>Paper# 154</b> | <b><i>Nanodisc-based approach to improve the distance measurement in membrane protein by spin-label ESR</i></b><br>Yun-Wei Chiang, National Tsing Hua University, Taiwan       |
| 15:30-15:45<br><b>Paper# 289</b> | <b><i>An integrated platform for the design, evaluation and production of recombinant protein constructs</i></b><br>Ming Wei Chen, Nanyang Technological University, Singapore |
| 15:45-16:00<br><b>Paper# 263</b> | <b><i>Monitoring of Hydrogenation by Benchtop NMR with Parahydrogen-Induced Polarization</i></b><br>Heelim Chae, Seoul Women's University, Korea                               |
| 16:00-16:20                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                       |

## QUANTITATIVE MRS/MRI

Chair/Co-Chair: S. Sendhil Velan / Dennis Hwang

|                                  |                                                                                                                                                                                                   |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 16:20-16:50<br><b>Paper# 109</b> | <b><i>Translational Metabolic Imaging of Obesity</i></b><br>S. Sendhil Velan, Singapore Bioimaging Consortium, A*STAR, Singapore                                                                  |
| 16:50-17:20<br><b>Paper# 204</b> | <b><i>The Metabolites Distribution and its Dynamical Process of Huntington's Disease Mice Model by Chemical Exchange Saturation Transfer Imaging</i></b><br>Dennis Hwang, Academia Sinica, Taiwan |
| 17:20-17:50<br><b>Paper# 260</b> | <b><i>Dynamic Causal Model Analysis on 7T fMRI Data of Major Depressive Disorder</i></b><br>Chaejoon Cheong, Korea Basic Science Institute, Korea                                                 |

**Saturday, 6 July 2019**

Venue: Plenary Lecture Hall (CR1)

## PLENARY LECTURES-5

Chair: **Jaume Torres**

|           |                                                                                                                                                 |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:00-9:40 | <b><i>Plenary Talk 5: “ Modify the Modifier, a Convolutd Tale of Ubiquitin ”</i></b><br>Professor Chun Tang, Chinese Academy of Sciences, China |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------|

Venue: Classroom 2 (CR2)

## BIOMOLECULAR STRUCTURE & FUNCTION-6/7

Chair: **Ping-Chiang Lyu**

|                                  |                                                                                                                                                                                    |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:50-10:20<br><b>Paper# 248</b>  | <b><i>Understanding the mechanism of small RNA mediated gene regulation in higher eukaryotes</i></b><br>Mandar V Deshmukh, CSIR - Centre for Cellular and Molecular Biology, India |
| 10:20-10:40                      | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                                           |
| 10:40-11:10<br><b>Paper# 270</b> | <b><i>High resolution protein 3D structure determination in living eukaryotic cell</i></b><br>Teppei Ikeya, Tokyo Metropolitan University, Japan                                   |
| 11:10-11:40<br><b>Paper# 118</b> | <b><i>The fundamental difference in Receptor-interacting protein kinase 3 (RIP3) amyloid structure between mouse and human</i></b><br>Junxia Lu, ShanghaiTech University, China    |
| 11:40-12:10<br><b>Paper# 252</b> | <b><i>In-cell NMR observation of the biological events within living cells</i></b><br>Noritaka Nishida, The University of Tokyo, Japan                                             |
| 12:10-12:25<br><b>Paper# 208</b> | <b><i>Solution structure and dynamics of anti-CRISPR protein AcrIIA4 reveals its recognition for binding interfaces of Cas9</i></b><br>Iktae Kim, Seoul National University, Korea |
| 12:35-13:00                      | Award / Closing (Plenary Lecture Hall , CR1)                                                                                                                                       |
| 13:00-14:00                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                        |

Venue: Classroom 3 (CR3)

### **METABOLOMICS –3**

Chair: **Ramakrishna V. Hosur**

|                                 |                                                                                                                                                         |
|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| 9:50-10:20<br><b>Paper# 282</b> | <b><i>Insights into the Metabolism of Lactobacillus plantarum B21 during industrial Processing</i></b><br>Oliver A.H. Jones, RMIT University, Australia |
| 10:20-10:40                     | Coffee / Tea Break (School of Biological Sciences Lobby)                                                                                                |

### **METHODS AND INSTRUMENTATION-3/ BIOMOLECULAR DYNAMICS-4**

Chair/Co-Chair: **Ramakrishna V. Hosur / Pramodh Vallurupalli**

|                                  |                                                                                                                                                                                          |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 285</b> | <b><i>Recent advances in NMR concerning the ease of use</i></b><br>Bjoern Heitman, Bruker Faellanden, Switzerland                                                                        |
| 11:10-11:40<br><b>Paper# 279</b> | <b><i>Studying Multi-State Protein Conformational Exchange using Double Resonance CEST Spectroscopy</i></b><br>Pramodh Vallurupalli, Tata Institute of Fundamental Research, India       |
| 11:40-12:10<br><b>Paper# 280</b> | <b><i>Herbolomics by NMR: A new frontier</i></b><br>Ramakrishna V Hosur, University of Mumbai, India                                                                                     |
| 12:10-12:25<br><b>Paper# 179</b> | <b><i>Expedited Protein Interaction via Engineered Target Search Pathways visualized by NMR Paramagnetic Relaxation Enhancement</i></b><br>So Young An, Seoul National University, Korea |
| 12:35-13:00                      | Award / Closing (Plenary Lecture Hall , CR1)                                                                                                                                             |
| 13:00-14:00                      | Lunch (School of Biological Sciences Lobby)                                                                                                                                              |

Venue: Classroom 4 (CR4)

## NATURE PRODUCT

Chair: **Shang-Te Danny Hsu**

|                                 |                                                                                                                                            |
|---------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------|
| 9:50-10:20<br><b>Paper# 145</b> | <b><i>Identification of individual compounds from NMR spectra of complex mixture</i></b><br>Kaifeng Hu, Chinese Academy of Sciences, China |
|---------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------|

|             |                                                          |
|-------------|----------------------------------------------------------|
| 10:20-10:40 | Coffee / Tea Break (School of Biological Sciences Lobby) |
|-------------|----------------------------------------------------------|

## MOLECULES IN MEDICINE / BIOMOLECULAR STRUCTURE & FUNCTION-8 / COMPUTATION IN NMR

Chair/Co-Chair: **Shang-Te Danny Hsu / Kaifeng Hu**

|                                  |                                                                                                                             |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| 10:40-11:10<br><b>Paper# 138</b> | <b><i>NMR-guided structure-based drug design for galectin inhibitors</i></b><br>Shang-Te Danny Hsu, Academia Sinica, Taiwan |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------|

|                                  |                                                                                                                                                                                                                                         |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 11:10-11:40<br><b>Paper# 290</b> | <b><i>Structure of G57W variant of human <math>\gamma</math>S-crystallin and its involvement in severe infantile cataracts</i></b><br>Kandala Venkata Ramana Chary, Indian Institute of Science Research and Education Berhampur, India |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

|                                  |                                                                                                                           |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------|
| 11:40-12:10<br><b>Paper# 291</b> | <b><i><sup>19</sup>F-NMR for Fragment-Based Drug Discovery</i></b><br>Chojiro Kojima, Yokohama National University, Japan |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------|

|                                  |                                                                                                                           |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------|
| 12:10-12:25<br><b>Paper# 218</b> | <b><i>Data Cleansing Strategy for Data Governance and Denoising in NMR</i></b><br>Shunji Yamada, Nagoya University, Japan |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------|

|             |                                              |
|-------------|----------------------------------------------|
| 12:35-13:00 | Award / Closing (Plenary Lecture Hall , CR1) |
|-------------|----------------------------------------------|

|             |                                             |
|-------------|---------------------------------------------|
| 13:00-14:00 | Lunch (School of Biological Sciences Lobby) |
|-------------|---------------------------------------------|

Thursday, 4 July 2019

13:10 - 14:00

Venue: School of Biological Sciences Lobby

|                              |                                                                                                                                                                                                                      |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 1<br/>ID: 101</b>  | <b><i>NMR resonance assignment of p50 subunit of NF-kappaB protein</i></b><br>Tahseen Raza, Indian Institute of Technology Roorkee, India                                                                            |
| <b>Poster 2<br/>ID: 102</b>  | <b><i>Study of Cyclic Heptapeptide Oral Bioavailability by NMR</i></b><br>Huy Ngoc Hoang, The University of Queensland, Australia                                                                                    |
| <b>Poster 3<br/>ID: 105</b>  | <b><i>NMR Characterization of Conformational Flexibility in Drosophila SUMO (dSmt3) and its Binding Surface for a SUMO Interaction Motif</i></b><br>Anupreet Kaur, Guru Nanak Dev University, India                  |
| <b>Poster 4<br/>ID: 106</b>  | <b><i>Solid State NMR Spectroscopy Studies the Nature of Structure Direction of OSDAs</i></b><br>Xiaolong Liu, Sun Yat-sen University, China                                                                         |
| <b>Poster 5<br/>ID: 107</b>  | <b><i>REAL-t1, An Effective Approach for Suppressing t1-noise in NMR Spectroscopy Based on Resampling algorithm</i></b><br>Bin Jiang, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, China |
| <b>Poster 6<br/>ID: 111</b>  | <b><i>Rational modulation of the enzymatic intermediates for tuning the phosphatase activity of HK853</i></b><br>Yixiang Liu, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, China         |
| <b>Poster 7<br/>ID: 113</b>  | <b><i>Study on the channel structure of type-FAU molecular sieve by 129Xe Solid-State NMR</i></b><br>Wei liu, Sinopec Shanghai Research Institute of Petrochemical Technology, China                                 |
| <b>Poster 8<br/>ID: 114</b>  | <b><i>Solid-State NMR study on the Effect of modified H-ZSM-5 on Methanol-To-Aromatics Conversion</i></b><br>Wei liu, Sinopec Shanghai Research Institute of Petrochemical Technology, China                         |
| <b>Poster 9<br/>ID: 115</b>  | <b><i>Solution Structure of the Antimicrobial Peptide S1-Nal-Nal in Complex with Lipopolysaccharide</i></b><br>Jyawei Cheng, National Tsing Hua University, Taiwan                                                   |
| <b>Poster 10<br/>ID: 119</b> | <b><i>Microsecond Timescale Dynamics of GDP-Bound Ras Underlies the Formation of Novel Inhibitor-Binding Pockets</i></b><br>Yunyun Mao, University of Science and Technology of China, China                         |
| <b>Poster 11<br/>ID: 121</b> | <b><i>1H NMR study of the relative arrangement between CTAB and TX-100 molecules in their mixed micelles</i></b><br>Shizhen Mao, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, China      |
| <b>Poster 12<br/>ID: 126</b> | <b><i>Characterization of microbial poly(<math>\gamma</math>-glutamic acid) and its polymer complex by solid NMR</i></b><br>Shiro Maeda, University of Fukui, Japan                                                  |
| <b>Poster 13<br/>ID: 127</b> | <b><i>Solution Structure, Dynamics and Function Investigation of Kringle Domain of Human ROR1</i></b><br>Kaifeng Hu, Kunming Institute of Botany, Chinese Academy of Science, China                                  |
| <b>Poster 14<br/>ID: 129</b> | <b><i>Annealing Effect on the Crystalline Phase of an Ethylene Ionomer investigated by Solid State NMR</i></b><br>Atsushi Asano, National Defense Academy, Japan                                                     |

|                              |                                                                                                                                                                                                                      |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 15<br/>ID: 132</b> | <b><i>Structural Basis of <math>\beta</math>-Methyl Epimerization by homodimeric enzyme MarH</i></b><br>Kaifeng Hu, Kunming Institute of Botany, Chinese Academy of Sciences, China                                  |
| <b>Poster 16<br/>ID: 134</b> | <b><i>Quantitative NMR Analysis of Dissolved Organic Molecules of Indoor Domestic Residuals</i></b><br>Khalid Salim AL Maqbali, Sultan Qaboos University, Oman                                                       |
| <b>Poster 17<br/>ID: 135</b> | <b><i>The Important Structural and Dynamic Features of Acyl Carrier Protein from <i>Thermotoga maritima</i> for its Hyperthermophilic Adaptation</i></b><br>Yeongjoon Lee, Konkuk University, Korea                  |
| <b>Poster 18<br/>ID: 136</b> | <b><i>Hsp33, an ATP-Independent Molecular Chaperone with Distinctive Dual Functions—Structural Identification of Holding and Unfoldase/Aggregase Activities</i></b><br>Chaeyeon Wang, Konkuk university, Korea       |
| <b>Poster 19<br/>ID: 137</b> | <b><i>Structure, Specificity, and Interaction of Propionibacterium acnes Acyl Carrier Protein with <math>\beta</math>-ketoacyl Acyl Carrier Protein Synthase III</i></b><br>Dasom Cheon, Konkuk University, Korea    |
| <b>Poster 20<br/>ID: 140</b> | <b><i>Investigation of Structural and Functional Relationship of Vaccinia Virus Envelope Protein A26 by NMR and SPR Spectroscopy</i></b><br>Kathleen Joyce Dela Rosa Carillo, National Chiao-tung University, Taiwan |
| <b>Poster 21<br/>ID: 142</b> | <b><i>Elimination of Background Signal by Phase-Incremented Pulses</i></b><br>Ling Wei, China University of Petroleum (East China), China                                                                            |
| <b>Poster 22<br/>ID: 152</b> | <b><i>Metabolic approach on infectious disease in White leg shrimp using HR-MAS NMR</i></b><br>Seohee Ma, Pusan National University, Korea                                                                           |
| <b>Poster 23<br/>ID: 155</b> | <b><i>NMR and SPR Investigation of Vaccinia Viral Protein H3</i></b><br>Gian Louis Buenavista Coronel, Academia Sinica, Taiwan                                                                                       |
| <b>Poster 24<br/>ID: 158</b> | <b><i>NMR Metabolomics based high throughput screening markers for whole body radiation exposure</i></b><br>Kiran Maan, Institute of Nuclear Medicine and Allied Sciences (INMAS), India                             |
| <b>Poster 25<br/>ID: 159</b> | <b><i>NMR-based Metabolomics Study on RBIV infection in Rock Bream</i></b><br>Seonghye Kim, Pusan National University, Korea                                                                                         |
| <b>Poster 26<br/>ID: 164</b> | <b><i>Rotational Motion of Molecules in Polar and Apolar Liquids: Implications for Spin Relaxation</i></b><br>Konstantin I. Momot, Queensland University of Technology, Australia                                    |
| <b>Poster 27<br/>ID: 169</b> | <b><i>In situ solid-state NMR of three-dimensionally magnetically oriented microcrystal suspension</i></b><br>Hiroshi Kadoma, Kyoto University, Japan                                                                |
| <b>Poster 28<br/>ID: 170</b> | <b><i>Structure and Dynamics studies on HIV-1 integrase catalytic core domain by NMR and XFEL</i></b><br>Jae-Hyun Park, Yonsei University, Korea                                                                     |
| <b>Poster 29<br/>ID: 171</b> | <b><i>NMR studies on Wnt/<math>\beta</math>-catenin and RAS-ERK pathways</i></b><br>Yunseok Heo, Yonsei University, Korea                                                                                            |
| <b>Poster 30<br/>ID: 172</b> | <b><i>ROS effects on NOX1 and catalase studied by NMR spectroscopy</i></b><br>Wonbin Lee, Yonsei University, Korea                                                                                                   |

|                              |                                                                                                                                                                                                            |
|------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 31<br/>ID: 173</b> | <b><i>Protein interactions between human chromatin remodeling components and tumor suppressor p53 by NMR spectroscopy</i></b><br>Taehee Kim, Yonsei University, Korea                                      |
| <b>Poster 32<br/>ID: 174</b> | <b><i>Structure and interaction studies on HIV-1 integrase/hSNF5</i></b><br>Jeongmin Han, Yonsei University, Korea                                                                                         |
| <b>Poster 33<br/>ID: 175</b> | <b><i>Separation of 2H solid-state NMR spectra assisted by molecular dynamics</i></b><br>Takahiro Iijima, Yamagata University, Japan                                                                       |
| <b>Poster 34<br/>ID: 178</b> | <b><i>The preparation of isotope labeled magnetite interacting sequences and the interaction with metal ions</i></b><br>Yi-Zong Lee, National Tsing Hua University, Taiwan                                 |
| <b>Poster 35<br/>ID: 181</b> | <b><i>Characering the mechanism of galectin-3-NTD self-association and liquid-liquid phase separation</i></b><br>Yi-Ping Chiu, National Yang-Ming university, Taiwan                                       |
| <b>Poster 36<br/>ID: 189</b> | <b><i>Mechanism of preferential NF-kappaB dimer formation as revealed by NMR spectroscopy</i></b><br>Manish Kumar, IIT-Roorkee, India                                                                      |
| <b>Poster 37<br/>ID: 191</b> | <b><i>NMR studies on molecular interaction between pro-matrix metalloproteinase-7 and syndecan-2</i></b><br>Ji-Hye Yun, Yonsei University, Korea                                                           |
| <b>Poster 38<br/>ID: 192</b> | <b><i>JH-H coupling Splitting Patterns and Subspectra Resolved from Steroidal Compounds</i></b><br>Dan Ni Wu, Institute of Chemistry, Academia Sinica, Taiwan                                              |
| <b>Poster 39<br/>ID: 193</b> | <b><i>Characterizing the structure and dynamics of the intrinsically disordered domain of Musashi-1</i></b><br>Tsai-Chen Chen, National Yang-Ming University, Taiwan                                       |
| <b>Poster 40<br/>ID: 195</b> | <b><i>H-NMR lipid profiles of human red blood cells with heart failure</i></b><br>Ming-Tong Tsau, Chang Gung University, Taiwan                                                                            |
| <b>Poster 41<br/>ID: 196</b> | <b><i>Vaccinia virus A26-G9 protein interaction and pH sensing regulating host cell entry pathway</i></b><br>Petra Sterbova, Academia Sinica, Taiwan                                                       |
| <b>Poster 42<br/>ID: 197</b> | <b><i>Extending the Lifetime of Native GTP-Bound Ras for Site-Resolved NMR Measurements: Quantifying the Allosteric Dynamics</i></b><br>Xiaomin Chen, University of Science and Technology of China, China |
| <b>Poster 43<br/>ID: 199</b> | <b><i>3D-HR-CSI-MOSY: Mobility Encoded Spectroscopy for Position-specific Metabolic Profiling of Intact Tissue</i></b><br>Kengo Ito, RIKEN, Japan                                                          |
| <b>Poster 44<br/>ID: 200</b> | <b><i>Probing Transient Release of Membrane-Sequestered ITT Motif of B cell receptor by Solution NMR Spectroscopy</i></b><br>Hui Wang, University of Science and Technology of China, China                |

|                              |                                                                                                                                                                                                                           |
|------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 45<br/>ID: 201</b> | <b><i>Probe the Conformation Change of Native Yeast Cytochrome c by Selective Detection of the Modified Methyl Groups</i></b><br>Xu Zhang, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, China |
| <b>Poster 46<br/>ID: 202</b> | <b><i>Structural Identification of a Purine/Pyrimidine Nucleoside Phosphorylase Activity of a Cupin-family Protein, YaiE</i></b><br>Sung-Hee Lee, Chungbuk National University, Korea                                     |

Friday, 5 July 2019

13:10 - 14:00

Venue: School of Biological Sciences Lobby

|                              |                                                                                                                                                                                                                                                                                     |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 47<br/>ID: 203</b> | <b><i>Structural aspects of a molten globular TgPDCD5 (host cellular programmed cell death-related protein) from pathogenic protozoan Toxoplasma gondii</i></b><br>Meng Hsuan Lin, National Taiwan University, Taiwan                                                               |
| <b>Poster 48<br/>ID: 205</b> | <b><i>Biophysical analysis on molecular interaction of monocyte chemoattractant protein with flavonoid baicalin</i></b><br>Nidhi Joshi, IIT roorkee, India                                                                                                                          |
| <b>Poster 49<br/>ID: 207</b> | <b><i>Characterizing the binding between CXCR3 and multiple ligands by NMR</i></b><br>Ya-Hsin Liu, National Tsing Hua University, Taiwan                                                                                                                                            |
| <b>Poster 50<br/>ID: 209</b> | <b><i>Acidosis imaging of skeletal muscles by chemical exchange saturation transfer (CEST) imaging</i></b><br>Yu-Wen Chen, Academia Sinica, Taiwan                                                                                                                                  |
| <b>Poster 51<br/>ID: 211</b> | <b><i>Structure and dynamic Features of human ACP and Bacterial ACPs and Their Interactions with FAS Proteins Studied by NMR Spectroscopy</i></b><br>Jungwoo Park, Konkuk University, Korea                                                                                         |
| <b>Poster 52<br/>ID: 212</b> | <b><i>Applications of magnetically oriented microcrystal array and suspension to analysis of anisotropic interactions</i></b><br>Ryosuke Kusumi, Kyoto University, Japan                                                                                                            |
| <b>Poster 53<br/>ID: 213</b> | <b><i>Machine-learning Based Growth Modeling of Fishes and Integrated Analysis of NMR Profiles and Environmental Factors</i></b><br>Taiga Asakura, RIKEN Center for Sustainable Resource Science, Yokohama, Japan                                                                   |
| <b>Poster 54<br/>ID: 214</b> | <b><i>The structural based analysis of fragmented human membrane protein CD44 and its communication with other proteins using solution NMR</i></b><br>Dong-Hoon KANG, Chungbuk National University, Korea                                                                           |
| <b>Poster 55<br/>ID: 215</b> | <b><i>Structural analysis about human membrane protein Caveolin 3</i></b><br>yu-bin Ma, Chungbuk National University, Korea                                                                                                                                                         |
| <b>Poster 56<br/>ID: 219</b> | <b><i>Increased Intestinal permeability in patients with Acute-on Chronic Liver failure (ACLF) and its recovery by dietary probiotic revealed by NMR based Urinary profiling of Lactulose Mannitol Ratio (LMR)</i></b><br>Umesh Kumar, Centre of Biomedical Research Lucknow, India |
| <b>Poster 57<br/>ID: 221</b> | <b><i>Developing endogenous brain protein L-PGDS as a magnetic resonance based diagnostic tool for amyloid detection in Alzheimer's disease</i></b><br>Bhargy Sharma, Nanyang Technological University, Singapore                                                                   |
| <b>Poster 58<br/>ID: 224</b> | <b><i>NMR Study of Cooperative DNA Binding of Transcription Factor MEIS1</i></b><br>Seo-Ree Choi, Gyeongsang National University, Korea                                                                                                                                             |
| <b>Poster 59<br/>ID: 225</b> | <b><i>NMR study of Intermolecular interaction of Transcription Factor DLX3 with Its target DNA</i></b><br>Ho-Seong Jin, Gyeongsang National University, Korea                                                                                                                       |

|                              |                                                                                                                                                                                                                            |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 60<br/>ID: 226</b> | <b><i>Hydrogen Exchange NMR Study of HOXB13 consensus DNA duplexes</i></b><br>Hansol Choi, Gyeongsang National University, Korea                                                                                           |
| <b>Poster 61<br/>ID: 227</b> | <b><i>Structure and molecular association of the full-length Aux/IAA17 for the auxin-response transcriptional regulation in plants</i></b><br>Youngim Kim, Seoul National University, Korea                                |
| <b>Poster 62<br/>ID: 228</b> | <b><i>Paramagnetic NMR-based structural analysis of linear diubiquitin in solution</i></b><br>Xueni Hou, Kyoto University, Japan                                                                                           |
| <b>Poster 63<br/>ID: 229</b> | <b><i>NMR Dynamics study of Transcription Factor FLI1 complexes with its target DNA</i></b><br>Na-hyun Kim, Gyeongsang National University, Korea                                                                          |
| <b>Poster 64<br/>ID: 230</b> | <b><i>Structural significance of CCL5 conserved FAY sequence</i></b><br>Jin-Ye Li, National Tsing Hua University, Taiwan                                                                                                   |
| <b>Poster 65<br/>ID: 231</b> | <b><i>Structural study of the interaction between C-terminal domain of IP3 receptor and Huntingtin proteins</i></b><br>Ha-Neul Kim, Ajou university, Korea                                                                 |
| <b>Poster 66<br/>ID: 232</b> | <b><i>Investigation of protein binding between E3 ligase RNF126 and ubiquitin</i></b><br>Ji-Na Yoo, Ajou university, Korea                                                                                                 |
| <b>Poster 67<br/>ID: 234</b> | <b><i>Mechanism of amyloid-<math>\beta</math> chaperone activity of Lipocalin type prostaglandin D synthase</i></b><br>Bhuvaneswari Kannaian, Nanyang Technological University, Singapore                                  |
| <b>Poster 68<br/>ID: 235</b> | <b><i>Cloning and Backbone Assignment of Novel Acyl Carrier Protein from Acinetobacter baumannii</i></b><br>Sungjae Choi, Konkuk University, Korea                                                                         |
| <b>Poster 69<br/>ID: 236</b> | <b><i>Solid-state NMR Investigation on the Structure of Histones in the Nucleosome</i></b><br>Chinmayi Prasanna, Nanyang Technological University, Singapore                                                               |
| <b>Poster 70<br/>ID: 237</b> | <b><i>Systematic engineering of E. coli to exhibit magnetic properties</i></b><br>Rupali Reddy Pasula, Nanyang Technological University, Singapore                                                                         |
| <b>Poster 71<br/>ID: 238</b> | <b><i>Rational design of chitinase to enhance chitio-oligosaccharide productivity</i></b><br>I-Chuan Chou, National Tsing Hua University, Taiwan                                                                           |
| <b>Poster 72<br/>ID: 239</b> | <b><i>Structural Basis For DNA Recognition And Transduction Activation By The Response Regulator OmpR</i></b><br>Sushant Sadotra, Institute of Biomedical Sciences, Academia Sinica, Taiwan                                |
| <b>Poster 73<br/>ID: 240</b> | <b><i>Distinctive metabolic Signatures of Systemic lupus erythematosus and TAKAYASU Arteritis revealed by <sup>1</sup>H NMR based serum metabolomics</i></b><br>Nikhil Gupta, Centre of Biomedical Research Lucknow, India |
| <b>Poster 74<br/>ID: 242</b> | <b><i>Quantitative NMR Analysis of Dissolved Organic Molecules of Indoor Domestic Residuals</i></b><br>Ahoud Ibrahim AL Naamani, Sultan Qaboos University, Oman                                                            |

|                              |                                                                                                                                                                                                                                                                            |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 75<br/>ID: 243</b> | <b><i>Cloning, Purification, and Labeling of antimicrobial peptide Papiliocin</i></b><br>Kkabi Son, Konkuk University, Korea                                                                                                                                               |
| <b>Poster 76<br/>ID: 244</b> | <b><i>Conformational dynamics of Rous Sarcoma Virus capsid protein visualized with conjoint use of NMR and single molecule FRET</i></b><br>Wenxue Jiang, Wuhan institute of physics and mathematics, China                                                                 |
| <b>Poster 77<br/>ID: 246</b> | <b><i>A<math>\beta</math>42 Peptide Functionalized Iron Oxide Nanoparticles for Specific Targeting of SH-SY5Y Neuroblastoma Cells</i></b><br>Yang Xia, Nanyang Technological University, Singapore                                                                         |
| <b>Poster 78<br/>ID: 249</b> | <b><i>NMR structural study of Nor1, an orphan nuclear receptor</i></b><br>Jun Yeob Yoo, Nanyang Technological University, Singapore                                                                                                                                        |
| <b>Poster 79<br/>ID: 253</b> | <b><i>Structural Studies of Tri-loop Interaction in DUSP22</i></b><br>Chih-Hsuan Lai, National Tsing-Hua University, Taiwan                                                                                                                                                |
| <b>Poster 80<br/>ID: 254</b> | <b><i>NMR study of CXCR3 extracellular elements binding chemokine ligands, CXCL4/CXCL4L1</i></b><br>Eh-Tzen Lee, National Tsing-Hua University, Taiwan                                                                                                                     |
| <b>Poster 81<br/>ID: 258</b> | <b><i>Structural Engineering of Hybrid Organic-Inorganic Perovskites Based on Imidazolium-Type Cations</i></b><br>Walter P. D. Wong, Nanyang Technological University, Singapore                                                                                           |
| <b>Poster 82<br/>ID: 259</b> | <b><i>Using SSNMR to Characterise Platinum Nanoparticles Capped with Isolated Zinc Species in SBA-15 Channels</i></b><br>Benjamin Elias Griffith, University of Warwick, United Kingdom                                                                                    |
| <b>Poster 83<br/>ID: 261</b> | <b><i>Rejection of Lateral Clam Shell Model for Fatty Acids to Enter into Human Intestinal Fatty-Acid Binding Protein</i></b><br>Yimei Lu, National University of Singapore, Singapore                                                                                     |
| <b>Poster 84<br/>ID: 262</b> | <b><i>A MAS NMR and Diffraction Study of Cis/Trans Polymeric Materials</i></b><br>Nicole Louise Kelly, University of Warwick, United Kingdom                                                                                                                               |
| <b>Poster 85<br/>ID: 264</b> | <b><i>The SABRE for the polarization of Di-(2-picoly)amine</i></b><br>Sein Min, Seoul Women's University, Korea                                                                                                                                                            |
| <b>Poster 86<br/>ID: 265</b> | <b><i>A Solid State NMR and Powder XRD Study of the Phase Evolution in the Mixed-Occupancy Csx(CH<sub>3</sub>NH<sub>3</sub>)<sub>1-x</sub>PbX<sub>3</sub> Hybrid Lead Halide Perovskite System</i></b><br>Sai S.H. Dintakurti, Nanyang Technological University, Singapore |
| <b>Poster 87<br/>ID: 266</b> | <b><i>Mechanism of inhibition of chaperone protein LPGDS by anticholinergic drugs</i></b><br>Kimberly Jia Yi Low, Nanyang Technological University, Singapore                                                                                                              |
| <b>Poster 88<br/>ID: 267</b> | <b><i>Investigation of the modulation of native client protein dynamics and activities by chaperone Hsp70</i></b><br>Lichun He, Wuhan Institute of Physics and Mathematics, China                                                                                          |
| <b>Poster 89<br/>ID: 268</b> | <b><i>The Role of Acetyl coenzyme A in Progressing the Catalytic Cycle of Insect Arylalkylamine N-acetyltransferase</i></b><br>Chu-Ya Wu, National Tsing Hua University, Taiwan                                                                                            |

|                              |                                                                                                                                                                   |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Poster 90<br/>ID: 274</b> | <b><i>High-pressure NMR study of the locally disordered conformation of outer surface protein A (OspA)</i></b><br>Takuro Wakamoto, Ritsumeikan University, Japan  |
| <b>Poster 91<br/>ID: 278</b> | <b><i>Functional details of the toxin-antitoxin system based on a structural study</i></b><br>Sung-Min Kang, Seoul National University, Korea                     |
| <b>Poster 92<br/>ID: 294</b> | <b><i>Towards a realistic molecular model of a highly glycosylated receptor-like protein tyrosine phosphatase</i></b><br>Yong-Sheng Wang, Academia Sinica, Taiwan |