**Conference Program：**

First Day

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| 2018.5.4 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
| 8:00-8:45 |  | Conference Registration |  |  |
| 8:45-9:00 | 15 | Opening Ceremony |  |  |
| Plenary Lecture | | | | |
| Chair: | Gerrit Schüürmann | 9:00-10:10 |  |  |
| 9:00-9:35 | 35 | VEGAHUB: introducing a new platform for read across, QSAR and prioritization | Benfenati, Emilio | Department of Environment and Health Sciences, Istituto di Ricerche Farmacologiche Mario Negri, *Italy* |
| 9:35-10:10 | 35 | Computational methods for supporting risk assessment of ionic liquids | Puzyn, Tomasz | Faculty of Chemistry, University of Gdansk, *Poland* |
| 10:10-10:25 |  | Coffee Break |  |  |
| 2018.5.4 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
|  |  | Session I - 1: Computational Toxicology |  |  |
| Chair: | Ito Chao | 10:25-12:05 |  |  |
| 10:25-10:50 | 25 | Virtual screening of InterBioScreen natural database in search of multi-target leads against Alzheimer’s disease | Roy, Kunal | Department of Pharmaceutical Technology, Jadavpur University, *India* |
| 10:50-11:15 | 25 | Free online Danish (Q)SAR predictions database with >600,000 substances | Wedebye, Eva Bay | Division of Diet, Disease Prevention and Toxicology, DTU Food, *Denmark* |
| 11:15-11:40 | 25 | Analysing differences of similar molecules for tuning QSAR and read-across results | Gini, Giuseppina | the Politecnico di Milano, *Italy* |
| 11:40-12:05 | 25 | An unified in silico model for probing the (eco-)toxicity of nanoparticles | Concu, Riccardo | REQUIMTE/Department of Chemistry and Biochemistry, University of Porto, *Portugal* |
| 12:05-13:30 |  | Lunch |  |  |
| 2018.5.4 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
|  |  | Session II: Environmental Computational Chemistry |  |  |
| Chair: | Fei Ding | 13:30-14:20 |  |  |
| 13:30-13:55 | 25 | A mechanistic understanding of heavy metals complexation on clay edge surfaces | Liu, Xiandong | School of Earth Sciences and Engineering, Nanjing University, *China* |
| 13:55-14:20 | 25 | Quantum chemical study on Criegee intermediate decay processes in the atmosphere | Takahashi, Kaito | Institute of Atomic and Molecular Sciences, *Taiwan* |
| 14:20-15:10 | 50 | Application of AI and machine learning to predictive toxicology and environmental science | Gini, Giuseppina  Tetko, Igor V.  Roy, Kunal | Talking Session |
| 15:10-15:25 |  | Coffee Break |  |  |
| 2018.5.4 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
| Chair: | Xiandong Liu | 15:25-17:05 |  |  |
| 15:25-15:50 | 25 | Heterogeneous nanomaterials Safer-by-design: towards computational characterization of novel TiO2-based photocatalyst | Mikolajczyk, Alicja | Laboratory of Environmental Chemometricsand Department of Environmental Technology, University of Gdansk, *Poland* |
| 15:50-16:15 | 25 | Mechanistic insights into molecular initiating event of the androgen receptor provide guidelines for toxicity screening and chemical synthesis | Shi, Wei | School of the Environment, Nanjing University, *China* |
| 16:15-16:40 | 25 | Rationalization and prediction of the impact of different metals on carbon dioxide emission from soil | Chang, Chia Ming | Department of Soil and Environmental Sciences, National Chung Hsing University, *Taiwan* |
| 16:40-17:05 | 25 | A study of toxicity of bio-molecules invoking conceptual density functional theory | Chakraborty, Tanmoy | Department of Chemistry, Manipal University Jaipur, *India* |
| 18:30-20:30 |  | Dinner Banquet Splendor Hotel (<http://splendor.ehosting.com.tw/>) |  |  |

Second Day

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| 2018.5.5 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
| Plenary Lecture | | | | |
| Chair: | Emilio Benfenati | 8:50-10:35 |  |  |
| 8:50-9:25 | 35 | Chemistry and our common future | Chao, Ito | Institute of Chemistry, Academia Sinica, *Taiwan* |
| 9:25-10:00 | 35 | Predictive assessment of the human and environmental toxicity of chemical substances | Schüürmann, Gerrit | Department of Ecological Chemistry, Head Helmholtz Centre for Environmental Research - UFZ Permoserstr. 15 04318 Leipzig, *Germany* |
| 10:00-10:35 | 35 | Progresses from health risk assessment to computational toxicology with revolutionary science advances | Wu, Kuen-Yuh | Legislator, Legislation Yuan, Taiwan & Institute of Occupational Medicine and Industrial Hygiene and Food Safety and Health, College of Public Health, National Taiwan University, *Taiwan* |
| 10:35-10:50 |  | Coffee Break |  |  |
| 2018.5.5 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
|  |  | Session I - 2: Computational Toxicology |  |  |
| Chair: | Kunal Roy | 10:50-12:05 |  |  |
| 10:50-11:15 | 25 | Impact of artificial intelligence and big data on ecotoxicology modeling | Tetko, Igor V. | Institute of Structural Biology, Helmholtz Zentrum Muenchen (GmbH), German Research Center for Environmental Health, *Germany* |
| 11:15-11:40 | 25 | A free online DTU QSAR predictor powered by Leadscope | Nikolov, Nikolai G. | Technical University of Denmark, National Food Institute, *Denmark* |
| 11:40-12:05 | 25 | Leveraging alternative assays for predicting skin sensitizers | Tung, Chun-Wei | School of Pharmacy and Ph.D. Program in Toxicology, Kaohsiung Medical University, *Taiwan* |
| 12:05-13:30 |  | Lunch |  |  |
| 2018.5.5 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
|  |  | Session III: Environmental Multimedia Model |  |  |
| Chair: | Tomasz Puzyn | 13:30-15:10 |  |  |
| 13:30-13:55 | 25 | BMC-SSD: an ecological risk assessment software based on species sensitivity distribution with Bayesian inference | He, Wei | School of Water Resources and Environment, China University of Geoscience, *China* |
| 13:55-14:20 | 25 | Uptake, distribution and transformation of iron nanoparticles in plants | Chang, Yoon-Seok | Division of Environmental Science and Engineering, Pohang University of Science and Technology (POSTECH), *Korea* |
| 14:20-14:45 | 25 | Investigation of ambient volatile organic compounds in primary schools: concentrations and health risk assessment | Wang,  Yu-Chun | Department of Environmental Engineering, Chung Yuan Christian University, *Taiwan* |
|  |  | Session IV: Predictive Toxicology |  |  |
| 14:45-15:10 | 25 | Enantioselective recognition of isomeric phenylpyrazole insecticides by human nicotinic acetylcholine receptor: Mechanistic insights from static, dynamic enantiomeric behavior and structural flexibility | Ding, Fei | Department of Chemistry, China Agricultural University, *China* |
| 15:10-15:25 |  | Coffee Break |  |  |
| 2018.5.5 |  |  |  |  |
| Time | min | Speech Topic | Speaker |  |
| Chair: | Eva Bay Wedebye | 15:25-17:05 |  |  |
| 15:25-15:50 | 25 | Paraquat-induced oxidative injury in erythrocytes is associated with perturbations of essential metal level and antioxidant enzyme activity | Lin, Ming-Cheng | Department of Medical Laboratory Science and Biotechnology, Central Taiwan University of Science and Technology, *Taiwan* |
| 15:50-16:15 | 25 | TOXIOMICS model application for chronic exposure to NOAEL dosage of DEHP and its metabolite, MEHP promote ovary carcinogenicity and reproductive toxicity with up-regulation of ARNT mechanism | Chao, Ming-Wei | Department of Bioscience Technology, Chung Yuan Christian University, *Taiwan* |
| 16:15-16:40 | 25 | Evaluating ecotoxicological risk of illicit drugs by exploring their toxic mechanisms in medaka fish (Oryzias latipes) under environmentally relevant exposures | Chen, Pei-Jen | Department of Agricultural Chemistry, National Taiwan University, *Taiwan* |
| 16:40-17:05 | 25 | Design simple and cost effective devices to measure heartbeat, blood flow, swimming activity and behavior to evaluate the potential chemical toxicity in Zebrafish | Hsiao, Chung-Der | Department of Bioscience and Technology, Chung Yuan Christian University, *Taiwan* |
| 17:05-17:30 | 25 | Closing Ceremony |  |  |

Third Day

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| 2018.5.6 |  |  |  |  |
| Time |  |  |  |  |
| 08:30-15:30 |  | One Day Tour |  |  |