Monday, 11th June 2018

14:00 – 20:00	**Registration**
15:00 – 17:00	**QsarDB workshop – Using and authoring content for the QsarDB** *The workshop will focus on creating content on the QsarDB repository (http://qsardb.org/). Participants will get an interactive guide on how to organize their QSAR/QSPR data and models, how to upload (i.e. publish) model archives to the QsarDB and use predictive models with QsarDB web applications. General QSAR aspects will be covered with emphasis on the open data approach on presentation of data sets and predictive models, as well as on best practices for conducting reproducible QSAR research.*
17:30 – 18:00	**Opening ceremony**
Opening lectures	*Chair: Mark Cronin*
18:00 – 18:45	**Chemometric QSAR modelling for hazard assessment and priority setting of environmental pollutants** *Paola Gramatica (University of Insubria, Italy)*
18:45 – 19:00	***History of QSAR workshops*** *Uko Maran, Klaus Kaiser (to be ammended)*
19:30 – 21:00	**Welcome reception**

Tuesday, 12th June 2018

8:00 – 9:00	**Registration**
Session 1: (Q)SAR models for regulatory use	
Keynote lecture	*Chairs: Romualdo Benigni, Marjan Vračko*
9:00 – 9:40	**Better read-across: improving *in silico* predictions with 21st century toxicology new approach methodologies** *Mark Cronin (Liverpool John Moores University, UK)*
Oral communications	
9:40 – 10:00	**(Q)SARs as adaptations to REACH information requirements** *Andrea Gissi (ECHA, Finland)*
10:00 – 10:20	**Ten years history of the OECD QSAR Toolbox** *Terry W. Schultz (University of Tennessee, USA)*

10:20 – 10:40	**Successes of international collaboration on the OECD QSAR toolbox. Lessons learned and vision for future** *Eeva Leinala (OECD - Environment, Health and Safety Division, France)* *Tomasz Sobanski (ECHA, Finland)*
10:40 – 11:00	**Coffee break**
Oral communications	*Chairs: Kannan Krishnan, Andrzej Szymoszek*
11:00 – 11:20	**Moving towards incorporation of QSARs in defined approaches for potential test guidelines** *Patience Browne (OECD - Environment, Health and Safety Division, France)*
11:20 – 11:40	**Availability and applicability of computational approaches for the safety assessment of nanomaterials** *Andrea-Nicole Richarz (EC Joint Research Centre, Italy)*
11:40 – 12:00	**Making the prediction of the AMES test useful for industry: a combined approach** *Giuseppina Gini (Politecnico di Milano, Italy)*
12:00 – 12:20	**Ames/QSAR international collaborative project** *Masamitsu Honma (National Institute of Health Sciences, Japan)*
12:20 – 12:40	**High-throughput screening of azo-based substances in the Australian Inventory of Chemical Substances (AICS)** *Anna Cruz (Australian Government Department of Health, Australia)*
12:40 – 13:00	**QSAR models to predict properties of dyes for regulatory use** *Davide Ballabio (University of Milano - Bicocca, Italy)*
13:00 – 14:00	**Lunch**
Keynote lecture	*Chairs: Emilio Benfenati, Andrea Gissi*
14:00 – 14:40	***In silico* toxicology protocols** *Glenn Myatt (Leadscope, USA)*
Oral communications	
14:40 – 15:00	**The current application state of QSARs in Chinese enterprises: Opportunities and challenges** *Max Liu (Hangzhou Jireh Standard Co., China)*
15:00 – 15:20	**The use of *in silico* methods to support regulatory decisions in various regulatory frameworks** *Antje Gerloff-Elias (Dr. Knoell Consult, Germany)*
15:20 – 15:40	**QSARs for thiochemicals – a case study of using alternative information for REACH registrations** *Monika Nendza (Analytical Laboratory, Germany)*
15:40 – 16:00	***In chemico* thiol reactivity and aquatic toxicity of potential bi-functional reactive esters** *Terry W. Schultz (University of Tennessee, USA)*
16:00 – 16:30	**Coffee break & Posters**

Oral communications	*Chairs: Andrea-Nicole Richarz, Ester Papa*
16:30 – 16:50	**ADs and DAs** *David A. Bofill (EC Joint Research Centre, Italy)*
16:50 – 17:10	**Evaluation of the applicability of existing QSAR models for predicting the genotoxicity of pesticides and their metabolites** *Romualdo Benigni (Alpha-Pretox, Italy)*
17:10 – 17:30	**Analogue approach according to the requirements as laid down in the RAAF (Read-Across Assessment Framework)** *Andrzej Szymoszek (Dr. Knoell Consult, Germany)*
17:30 – 18:30	**Poster session**

Wednesday, 13th June 2018

8:00 – 10:00	**Workshop ExCAPE (Exascale Compound Activity Prediction Engine): HPC session** *HPC-as-a-Service continues to lower the entry barrier for users who are interested in utilizing massive parallel computers for modeling. This workshop will introduce a drug discovery web platform together with a platform for defining and executing scientific pipelines - HyperLoom that enable large-scale end-to-end machine learning applications being executed on supercomputing facilities via HPC as a Service Middleware. A participant will see general introduction to the platform and live examples.*

Session 2: Models for human health effects

Keynote lecture	*Chairs: Uko Maran, Janez Mavri*
10:00 – 10:40	**2D and 3D structure-activity modeling of mosquito repellents: a review** *James Devillers (CTIS, France)*
10:40 – 11:00	**Coffee break & Posters**
Oral communications	
11:00 – 11:20	**Mitochondrial dysfunction: mechanisms, structure-activity and cardiotoxicity** *Steven Enoch (Liverpool John Moores University, UK)* *Terry W. Schultz (University of Tennessee, USA)*
11:20 – 11:40	**Molecular signatures as biomarker of exposure in systems toxicology: crowd-sourced verification of computational methods and data applied to a heat-not-burn candidate modified risk tobacco product** *Florian Martin (Philip Morris Products S.A., Switzerland)*
11:40 – 12:00	***In vitro* vs. *in vivo* metabolism: comparative analysis and simulation** *Petko I. Petkov ("Prof. Assen Zlatarov" University, Bulgaria)*
12:00 – 12:20	**High-throughput pharmacokinetics for drug discovery** *Robert D. Clark (Simulations Plus, USA)*
12:20 – 12:40	**Kinetic model for simulating skin metabolism: Pre-validation** *Hristiana Ivanova ("Prof. Assen Zlatarov" University, Bulgaria)*
12:40 – 14:00	**Lunch**

Keynote lecture	*Chairs: James Devillers, Katja Venko*
14:00 – 14:40	**Thresholds of Toxicological Concern (TTC): development and use in occupational health risk assessment** *Kannan Krishnan (IRSST, Canada)*
Oral communications	
14:40 – 15:00	**An *in silico* screening strategy to evaluate toxicological properties of 20,000 cosmetic ingredients of plant extracts** *Alessandra Roncaglioni (IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Italy)*
15:00 – 15:20	**A tiered approach for screening chemicals for biomagnification potential in humans** *Alessandro Sangion (University of Insubria, Italy)*
15:20 – 15:40	**Classification models for pH-permeability profile to describe regional based absorption in gastrointestinal tract** *Mare Oja (University of Tartu, Estonia)*
15:40 – 16:00	**Integration of *in silico* models to establish level of safety concern for food contact chemicals** *Serena Manganelli (IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Italy)*
16:00 – 16:30	**Coffee break & Posters**
16:30 – 18:30	**Guided tour to castle Bled**
19:30	**GALA DINNER**

Thursday, 14th June 2018

8:00 – 10:00	**Workshop ExCAPE (Exascale Compound Activity Prediction Engine): Machine learning session** *Multi-task machine learning drew significant attention to the QSAR community in the past years, especially with a wave of deep learning publications. In this workshop, we will introduce an 'easy' alternative to deep learning: a multi-task Bayesian matrix factorization with side information – SMURFF with examples in Jupyter notebooks. SMURFF provides flexible pipeline for building large scale QSAR model that can be used both on a personal computer and deployed on HPC environment: https://github.com/exascience/smurff*

Session 3: Models for ecotoxicological and environmental effects

Keynote lecture	*Chairs: Alessandra Roncaglioni, Marjan Tušar*
10:00 – 10:40	**QSAR model presentation and reporting: physical and chemical properties, ecotoxic, environmental fate, human health and toxico-kinetics endpoints** *Uko Maran (University of Tartu, Estonia)*
10:40 – 11:00	**Coffee break & Posters**
Oral communications	
11:00 – 11:20	**Fish early-life stage toxicity predicted from acute *Daphnia magna* toxicity and molecular descriptors** *Ayako Furuhama (NIES - National Institute for Environmental Studies, Japan)*

11:20 – 11:40	**Identifying active pharmaceutical ingredients exhibiting excess toxicity in environmental species** *Madden Judith (Liverpool John Moores University, UK)*
11:40 – 12:00	**QSAR prediction of biotransformation half-lives and application for PBT assessment refinement** *Ester Papa (University of Insubria, Italy)*
12:00 – 12:20	**CATALOGIC 301C model – validation and improvement** *Irina Dermen ("Prof. Assen Zlatarov" University, Bulgaria)*
12:20 – 12:40	***Prediction of freshwater algal and planarian toxicity of contaminants with no ecotoxicological data*** *Melek Türker Saçan (Bogazici University, Turkey)*
12:40 – 14:00	**Lunch**

Session 4: Protein-ligand interactions, *in silico* studies related to toxicological effects

Keynote lecture	*Chairs: Roberto Todeschini, Marjana Novič*
14:00 – 14:40	**Use of mathematical descriptors and robust statistical methods in predicting mutagenicity of congeneric and diverse sets of chemicals** *Subhash C. Basak (University of Minnesota Duluth, USA)*
Oral communications	
14:40 – 15:00	**Large scale protein-ligand interaction prediction using Bayesian matrix factorization with side information: comparison with single task models** *Vladimir Chupakhin (Janssen Pharmaceutica NV, Belgium)*
15:00 – 15:20	**The effect of rational selection of training sets from an imbalanced AhR activation dataset on QSAR models accuracy and applicability domain coverage for a large set of REACH substances** *Kyrylo O. Klimenko (Technical University of Denmark, Denmark)*
15:20 – 15:40	**How many proteins a ligand can bind?** *Elena Lo Piparo (Nestlé Research Center, Switzerland)*
15:40 – 16:00	**Mechanistic interpretation of neural network models for characterization of binding activity of fullerene derivatives** *Natalja Fjodorova (National Institute of Chemistry, Slovenia)*
16:00 – 16:30	**Coffee break & Posters**
Oral communications	*Chairs: Petko I. Petkov, Melek Türker Saçan*
16:30 – 16:50	**Application of bioactivity profile based fingerprints for building machine learning models** *Noé J. Sturm (AstraZeneca, Sweden)*
16:50 – 17:10	**Comparison of computational tools and informatics workflows for the identification of read-across analogues** *Mark Cronin (Liverpool John Moores University, UK)*

17:10 – 17:30	**Read-across for the safety assessment of nanomaterials: possible approaches, challenges and perspectives** *Agnieszka Gajewicz (University of Gdansk, Poland)*
17:30 – 17:50	**Assessing the genotoxicity of pesticides metabolites through Read Across: case studies** *Cecilia Bossa (Istituto Superiore di Sanità, Italy)*
17:50 – 18:10	**QSAR analysis of bisphenol-A and bisphenol replacements** *Otakuye Conroy-Ben (Arizona State University, USA)*

Friday, 15th June 2018

Session 5: Software and tools

Keynote lecture	*Chairs: Paola Gramatica, Glenn Myatt*
9:00 – 9:40	**Prioritization of chemical substances for PBT, CMR and endocrine disrupting activity: the JANUS system** *Emilio Benfenati (IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Italy)*
Oral communications	
9:40 – 10:00	**Correct splits for cross- and test validation. Is there any difference among leave-many-out variants?** *Károly Héberger (Hungarian Academy of Sciences, Hungary)*
10:00 – 10:20	**Detecting activity-rich structural regions by a new chemoinformatic approach: Mapping of Activity through Dichotomic Scores (MADS).** *Roberto Todeschini (University of Milano-Bicocca, Italy)*
10:20 – 10:40	**UVCBs: methodology for substance identification and application to fate and hazard assessment** *Stela Kutsarova ("Prof. Assen Zlatarov" University, Bulgaria)*
10:40 – 11:00	**Coffee break**
Oral communications	*Chairs: Natalja Fjodorova, Nikola Minovski*
11:00 – 11:20	**Introducing *ab initio* QSAR – a universal QSAR-based tool for regression and classification** *Kristijan Vukovic (IRCCS-Istituto di Ricerche Farmacologiche Mario Negri, Italy)*
11:20 – 11:40	**Utility of unsupervised machine learning from big data in QSAR** *Suman Chakravarti (MultiCASE Inc., USA)*
11:40 – 12:00	**Mechanistic 3D skin penetration model accounting for local inhomogene-ity, vehicle effects and skin variability by the COSMOperm method** *Johannes Schwöbel (COSMOlogic GmbH & Co., Germany)*
12:00 – 12:20	**Implementation of an OASIS pipeline prioritization scheme for GHS classification in Merck**

	Yoanna Todorova ("Prof. Assen Zlatarov" University, Bulgaria)
12:20 – 12:40	**New functionalities of the QSAR Toolbox: Category consistency and alert performance** *Chanita Kuseva ("Prof. Assen Zlatarov" University, Bulgaria)*
12:40 – 13:00	**Prediction of toxicity and comparison of alternatives using WebTEST (Web-services Toxicity Estimation Software Tool)** *Valery Tkachenko (Science Data Experts, USA)*
13:00	**Closing remarks**
12:00 – 14:00	**Lunch Box**