



QSAR2014 - Milan, June 16th-20th 2014
WORKSHOP PROGRAMME



MONDAY JUNE 16th, 2014

9:00	Workshop Registration (<i>only for participants to QsarDB course</i>)	
9:30 - 13:00	Half-day course	Course on QsarDB U. Maran (University of Tartu, Estonia)
14:00	Workshop Registration (<i>for all participants</i>)	
OPENING SESSION		
15:20 - 15:30	Opening words	E. Benfenati (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy)
15.30 - 16:10	Opening talk	Using Adverse Outcome Pathways to guide the design of computational models and integrated testing strategies for the hazard assessment of chemicals M. Whelan (EC Joint Research Centre, Italy)
16:10 - 16:50	Opening talk	Combining High-Throughput Screening and QSAR: Collaborative efforts to build models for the Estrogen Receptor and other receptor targets R. Judson (US Environmental Protection Agency, USA)
16:50 - 17:10	Coffee break	
SESSION 1: Perspectives on Adverse Outcome Pathways		
17:10 - 17:50	Plenary talk	Predicting Organ Level Toxicity: From Adverse Outcome Pathways to <i>In Silico</i> Tools for Prediction M.T.D. Cronin (Liverpool John Moores University, UK)
17:50 - 18:10	Oral communication	A step forward in read-across acceptance: Characterisation of uncertainties using a systematic framework and moving towards read-across enhancement using the AOP concept A. O. Aptula (SEAC, Unilever R&D, UK)
18:30 - 20:30	Welcome Dinner for all participants at Istituto Mario Negri	

TUESDAY JUNE 17th, 2014

SESSION 2: Defining uncertainty of QSAR models and improving their acceptability		
9:00 - 9:40	Plenary talk	The use (and non-use) of QSARs for assessing safer alternatives J. Tunkel (SRC Inc., USA)

9:40 - 10:00	Oral communication	Accessibility, traceability and reproducibility of QSAR-s U. Maran (University of Tartu, Estonia)
10:00 - 10:20	Oral communication	A quantitative weight-of-evidence approach for estimating uncertainty and integrating alerts, read-across and QSAR J.F. Rathman (Ohio State University, USA)
10:20 - 10:40	Oral communication	One is a Lonely Number – Using Statistical Confidence Scoring to Improve QSPR Modelling F.P. Steinmetz (Liverpool John Moores University, UK)
10:40 - 11:10	Coffee break, Posters ar up	
SESSION 3: Novel software and tools		
11:10 - 11:30	Oral communication	Chemical landscapes for safety assessment and compound selection N. Jeliaskova (Ideaconsult Ltd., Bulgaria)
11:30 - 11:50	Oral communication	Reshaped Sequential Replacement algorithm: an efficient approach to variable selection R. Todeschini (University of Milano-Bicocca, Italy)
11:50 - 12:10	Oral communication	Toolbox Phase 3 Development - New Perspectives T. Sobanski (ECHA, Finland)
12:10 - 12:30	Oral communication	QSARINS: a new software for the development, analysis and validation of MLR models and QSARINS-Chem: Insubria datasets and QSAR/QSPR models for environmental pollutants S. Cassani (University of Insubria, Italy)
12:30 - 12:50	Oral communication	A novel unsupervised method for reducing the dimensionality of large QSAR datasets D. Ballabio (University of Milano-Bicocca, Italy)
12:50 - 14:10	Lunch	
SESSION 4: Models for human health effects		
14:10 - 14:30	Oral communication	Model for Predicting Respiratory Sensitization - On-going Developments C. Kuseva (University "Prof. D-R Asen Zlatarov", Bulgaria)
14:30 - 14:50	Oral communication	Analysing the effect of data quality on the predictive performance of structural alerts for identifying drugs capable of inducing phospholipidosis K. R. Przybylak (Liverpool John Moores University, UK)
14:50 - 15:10	Oral communication	Extrapolation Workflow for Predicting Mutagenicity of Chemicals P. Petkov (University "Prof. D-R Asen Zlatarov", Bulgaria)
15:10 - 15:30	Oral communication	Applicability domain for mutagenicity models: an <i>a priori</i> approach, based on chemical classes R. Gonella Diaza (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy)
15:30 - 16:00	Coffee break + Posters	

16:00 - 18:00	Poster session and courses	Short course on ToxTree 16:15 – 17:00 N. Jeliaskova (Ideaconsult Ltd, Bulgaria) http://toxtree.sourceforge.net/
		Short course on VEGA 17:15 - 18:00 A. Manganaro (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy) http://www.vega-qsar.eu/

WEDNESDAY JUNE 18th, 2014

SESSION 5: Models for ecotoxicological and environmental effects		
9:00 - 9:40	Plenary talk	Structure-activity relationship (SAR) modeling of mosquito larvicides J. Devillers (CTIS, France)
9:40 - 10:00	Oral communication	Study of Influence of Oganochlorines on GABA-receptors to <i>Daphnia magna</i> V .Tonkopii (Russian Academy of Sciences, Russia)
10:00 - 10:20	Oral communication	Predictive QSAR Modeling for Toxicity of Ionic Liquids to <i>Daphnia magna</i>: Aromaticity vs. Lipophilicity K. Roy (Jadavpur University, India)
10:20 - 10:40	Oral communication	A QSAR Model For Acute Aquatic Toxicity Towards <i>Daphnia magna</i> M. Cassotti (University of Milano-Bicocca, Italy)
10:40 - 11:10	Coffee break + Posters	
11:10 - 11:30	Oral communication	Discriminating toxicant classes by mode of action: Baseline and excess toxicity M. Nendza (Analytisches Laboratorium, Germany)
11:30 - 11:50	Oral communication	Unsupervised Classification of Mechanisms of Action for Aquatic Toxicity of Benzenes T. Schultz (The University of Tennessee, USA)
11:50 - 12:10	Oral communication	State of the Art in Application of QSAR techniques for Predicting Mixture Toxicity in Environment Risk Assessment J. Kim (KIST Europe, Germany)
12:10 - 12:30	Oral communication	Classification models for the bio-concentration factor G. Piir (University of Tartu, Estonia)
12:30 - 14:00	Lunch	
SESSION 6: QSAR and REACH		
14:00 - 14:40	Plenary talk	Checking the applications of (Q)SAR approaches in the framework of the REACH regulation E. Mombelli (INERIS, France)
14:40 - 15:00	Oral communication	Development of software for REACH assessment of substances V. Drgan (National Institute of Chemistry, Slovenia)

15:00 - 15:20	Oral communication	Identification of structural alerts for reproductive and developmental toxicity for prioritization purposes A. Roncaglioni (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy)
15:20 - 15:40	Oral communication	Representation and Hazard Assessment of UVCB Substances D. Georgieva (University "Prof. D-R Asen Zlatarov", Bulgaria)
15:40 - 16:00	Coffee break + Posters	
16:00 - 16:40	Plenary talk	The use of QSARs under REACH after the second registration deadline M. Valentini (ECHA, Finland)
16:40 - 17:00	Oral communication	Prediction of thermal stability of organic compounds for REACH P. Rotureau (INERIS, France)
17:00 - 17:40	Round table	with regulators and industry representatives Confirmed participants <ul style="list-style-type: none"> • Marco Valentini - ECHA, Finland • Ralf Knauf - Centro REACH S.r.l., Italy • Enrico Mombelli - INERIS, France • Anna Böhnhardt - UBA, Germany
17:40 - 18:30	Poster session and courses	Short course on EPISuite J. Tunkel (SRC Inc., USA) http://www.epa.gov/oppt/exposure/pubs/episuite.htm

THURSDAY JUNE 19th, 2014

SESSION 7: QSAR and Cosmetics (I)		
9:00 - 9:40	Plenary talk	Prospects and Limitations of QSARs for Regulatory Use Q. Chaudhry (The Food & Environment Research Agency, UK)
9:40 - 10:00	Oral communication	Modeling in the Cosmetics Industry A. Detroyer (L'Oréal Paris, France)
10:00 - 10:20	Oral communication	Different approaches for modeling repeated dose toxicity F. Pizzo (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy)
10:20 - 10:40	Oral communication	New Computational Approaches for Repeated Dose Toxicity Prediction in view of the Safety Assessment of Cosmetic Ingredients A.N. Richarz (Liverpool John Moores University, UK)
10:40 - 11:00	Coffee break + Posters	
11:00 - 11:20	Oral communication	<i>In vitro</i> to <i>in vivo</i> extrapolation in the assessment of chemical safety – a case study on caffeine – containing cosmetics A. Paini (EC - JRC, Institute for Health & Consumer Protection, Italy)
SESSION 8: QSAR and Cosmetics (II)		
11:20 - 11:40	Oral communication	<i>In silico</i> Implementation of AOPs: Proof-of-concept Scheme for Skin Sensitization K. Gerova (University "Prof. D-R Asen Zlatarov", Bulgaria)

11:40 - 12:00	Oral communication	Electrophilic reactivity and skin sensitization potency of SNAr electrophiles D. W. Roberts (Liverpool John Moores University, UK)
12:00 - 12:20	Oral communication	Predicting skin phototoxicity from electronic transitions D. Asturiol (EC - JRC, Institute for Health & Consumer Protection, Italy)
12:20 - 12:40	Oral communication	Acute Oral Toxicity Modeling Accounting for Mechanism and Toxicological Mode of Action D. Nedelcheva (University "Prof. D-R Asen Zlatarov", Bulgaria)
12:40 - 14:00	Lunch	
SESSION 9: Exploring properties and effects relevant for human toxicity, relevant for cosmetics and other sectors		
14:00 - 14:20	Oral communication	New software to support read across, based on multiple profilers G. Gini (Politecnico di Milano, Italy)
14:20 - 14:40	Oral communication	Multi-scale modeling: prediction of in vivo hepatotoxicity from <i>in vitro</i> data S. Teng (INERIS, France)
14:40 - 15:00	Oral communication	The role of Transporters in the prediction of biliary excretion of compounds T. Ghafourian (Universities of Kent and Greenwich, UK)
SESSION 10: In silico strategies for food safety		
15:00 - 15:20	Oral communication	Integration of <i>in silico</i> models to establish safety concern of chemicals in food E. Lo Piparo (Nestlé Research Center, Switzerland)
15:20 - 15:40	Oral communication	QSAR screening of food contact material substances: Potential human health effects M. Dybdahl (Technical University of Denmark, Denmark)
15:40 - 16:10	Coffee break + Posters	
16:10 - 17:00	Round table	with regulators and industry representatives on QSAR for cosmetics Confirmed participants <ul style="list-style-type: none"> • Q. Chaudhry (The Food & Environment Research Agency, UK) • A. Richarz (Liverpool John Moores University, UK) • A. Detroyer (L'Oréal Paris, France) • L. Sousselier (UNITIS, France)
17:00 - 17:20	Student award election results	
17:20 - 17:30	Presentation of QSAR 2016	
17:30 - 18:15	Courses	Short course on VEGA Alberto Manganaro (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy) http://www.vega-qsar.eu/
20:00	Social dinner	

FRIDAY JUNE 20th, 2014

SESSION 11: NanoQSAR

9:00 - 9:40	Plenary talk	Nano-QSARs: challenges and opportunities R. Rallo (Universitat Rovira i Virgili, Catalunya)
9:40 - 10:00	Oral communication	Descriptors for NanoQSAR N. Golbamaki Bakhtyari (IRCCS - Istituto di Ricerche Farmacologiche "Mario Negri" Milano, Italy)
10:00 - 10:20	Oral communication	QSAR Studies of Nano Bio-Active Compounds Invoking DFT Based Quantum Mechanical Descriptors T. Chakraborty (Manipal University Jaipur, Rajasthan, India)
10:20 - 10:40	Oral communication	Nanoparticle toxicity vs electronic structure - a quantum chemical building block perspective G. Schüürmann (Helmholtz-Zentrum für Umweltforschung, Germany)
10:40 - 11:00	Coffee break	
SESSION 12: Modelling sophisticated properties of chemicals of biological interest		
11:00 - 11:20	Oral communication	Regression models based on molecular graphs for copper(II) binding to tetrapeptides containing histidyl residue N. Raos (Institute for Medical Research and Occupational Health, Croatia)
11:20 - 11:40	Oral communication	Molecular modelling of LXR binding in relation to the MoA/AOP framework for liver steatosis E. Fioravanzo (S-IN Soluzioni Informatiche srl, Italy)
11:40 - 12:00	Oral communication	hERG blocking of acids and zwitterions characterized by three thresholds for pKa, size and reactivity N. G. Nikolov (Technical University of Denmark, Denmark)
12:00 - 12:20	Oral communication	The Art and Science of Predicting Ionization Constants R. Fraczekwicz (Simulations Plus, USA)
12:20 - 12:40	Closing remarks	
12:40 - 14:00	Lunch	
14:00 - 17:00	Half-day course	Course on NanoQSAR Lang Tran (Institute of Occupational Medicine, Edinburgh, UK)