FINAL PROGRAMME
QSAR 2025 conference
3-6 June 2025, Milan, Italy

TUESDAY - 3 June 2025

TIME	SCHEDULE	PRESENTER	AFFILIATION
9,00 - 10,00	**Registration**		
10,00 - 10,20	**Opening remarks**		
	Methodological aspects of (Q)SARs modelling ***Section chairs: Kamel Mansouri & Emilio Benfenati***		
10,20 - 10,40	Quantitative read-across structure-activity relationship (q-RASAR) models for predictive toxicology	Kunal Roy	Drug Theoretics and Cheminformatics Laboratory, Jadavpur University, Kolkata, India
10,40 - 11,20	***Coffee Break***		
11,20 - 11,40	Coverage hierarchies of post-hoc ensemble models optimized for different goal functions	Nikolai G Nikolov	Technical University of Denmark, National Food Institute, Denmark
11,40 - 12,00	Kinetic in vitro Half-life model: A new formalism for toxicokinetic modelling	Atanas Chapkanov	Laboratory of Mathematical Chemistry, Burgas State University "Prof. D-r Assen Zlatarov", Burgas, Bulgaria
12,00 - 12,20	SkinSensDB 2.0: a comprehensive database of AOP assay data and transfer learning-based prediction model for skin sensitization	Fan Hoi-Ki	Department of Veterinary Medicine, National Taiwan University, Taipei, Taiwan
12,20 - 12,40	Predictive Modeling of Pesticides Reproductive Toxicity in Earthworms Using Interpretable Machine-Learning Techniques on Imbalanced Data	Mihkel Kotli	University of Tartu, Tartu, Estonia
12,40 - 13,00	The Development of In Silico Model for Skin Permeability with Consideration of Experimental Conditions	Yao-De Wang	Department and Graduate Institute of Veterinary Medicine, National Taiwan, University, Taipei, Taiwan
13,00 - 14,00	***Lunch***		
	AI, big data and QSAR ***Section chairs: Igor Tetko & Wei Shi***		
14,00 - 14,20	Development, Validation, and Application of a Human Reproductive Toxicity Prediction Model based on Adverse Outcome Pathway	Haoyue Tan	Nanjing University, Nanjing, China.
14,20 - 14,40	Exploring Graph Neural Network Architectures for QSAR	Alexander Dimitrios Kalian	King's College London, London, United Kingdom
14,40 - 15,00	How Chemical Language Models Learn: Architectural Insights into Molecular Structure and Chirality Recognition	Tadahaya Mizuno	The University of Tokyo, Tokyo, Japan
15,00 - 15,20	Development of Structural Alerts and Machine Learning Models to Predict Respiratory Irritation and Respiratory	Yaroslav Chushak	Human Performance Wing, Air Force Research Laboratory, Wright-Patterson AFB, USA
15,20 - 15,40	Optimization of parallel synthesis conditions with machine learning methods	Fabrizio Ambrogi	Selvita, Krakow, Poland
15,40 - 16,00	Mapping of reliability in predictions for QSAR consensus modelling	Davide Ballabio	Milano Chemometrics and QSAR research group, University of Milano-Bicocca, Milan, Italy
16,00 - 16,30	***Coffee break***		
16,30 - 18,00	**POSTER SESSION**		
18,00 - 18,30	KEYNOTE LECTURE Environmental Toxicology and Health: Knowledge-Driven Artificial Intelligence as an Effective Approach to Overcome the "Black Box" Dilemma	Wei Shi	Nanjing University, Nanjing, China
18,30 - 19,30	**Welcome reception**		

WEDNESDAY - 4 June 2025

TIME	SCHEDULE	PRESENTER	AFFILIATION
9,10 - 9,40	KEYNOTE LECTURE International collaborations and consensus modeling	Kamel Mansouri	NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM), NIEHS, NIH, RTP, NC
	Emerging technologies and challenges ***Section chairs: Davide Ballabio & Patrik Andersson***		
9,40 - 10,00	A Tiered Approach for Screening Chemicals for Biomagnification Potential in Air-Breathing Organisms	Alessandro Sangion	ARC - Arnot Research and Consulting, Toronto, ON, Canada
10,00 - 10,20	Federated Chemical Safety Assessment	Nicoleta Spînu	AI4Cosmetics, Amsterdam, The Netherlands
10,20 - 10,40	Status of NAMs based on machine learning and artificial intelligence approaches in regulatory toxicology	Sulev Sild	University of Tartu, Tartu, Estonia
10,40 - 11,20	***Coffee break***		
11,20 - 11,40	From prediction to decision: Guiding experts through complex weight-of evidence assessments	Adrian Fowkes	Lhasa Limited, Leeds, UK
11,40 - 12,00	On Applicability of Data-Driven Machine Learning Computational New Approach Methodologies for Hazard Identification in Chemicals Risk Assessment	Uko Maran	Institute of chemistry, University of Tartu, Tartu, Estonia
12,00 - 12,20	Exploiting Knowledge from Existing Physiologically-Based Kinetic Models to Improve Model Development	Alessio Gamba	Liverpool John Moores University, Liverpool, UK
12,20 - 14,20	***POSTER SESSION & LUNCH from 13,00***		
	In silico strategies for data poor endpoints or substances ***Section chairs: Ester Papa & Simona Kovarich***		
14,20 - 14,40	QSAR Models to Assess the Terrestrial Toxicity of Pharmaceuticals: A Starting Point for a Weight-of-Evidence Strategy	Erika Colombo	Mario Negri Institute for Pharmacological Research IRCCS - Laboratory of Chemistry and Environmental Toxicology, Milan, Italy
14,40 - 15,00	QSARs for the Prediction of the Human Transthyretin Binding Affinity of Per- and Polyfluoroalkyl Substances	Marco Evangelista	QSAR Research Unit in Environmental Chemistry and Ecotoxicology, University of Insubria, Varese, Italy
15,00 - 15,20	In silico prediction of repeat dose toxicity: A novel role of simulated metabolism	Chanita Kuseva	Laboratory of Mathematical Chemistry, Burgas State University "Prof. D-r Assen Zlatarov", Burgas, Bulgaria
15,20 - 15,40	In silico predictions for regulatory decision-making on agrochemicals: challenges and opportunities	Elena Lo Piparo	FMC, US
15,40 - 16,00	QSAR models to predict potency of tropane alkaloids against human muscarinic acetylcholine receptors	Arthur de Carvalho e Silva	University of Birmingham, Birmingham, UK
16,00 - 16,30	***Coffee break***		
	Drug design and Drug Toxicity ***Section chairs: Marjan Vračko & Elena Fioravanzo***		
16,30 - 16,50	Analysis of Tox24 challenge results	Igor V. Tetko	Helmholtz Zentrum München, Neuherberg, Germany
16,50 - 17,10	Whether endocrine disrupting effects require consideration of dimerization: ERα and AR give different answers	Jin Jin sha	State Key Laboratory of Pollution Control and Resource Reuse, School of the Environment, Nanjing University, Nanjing, China.
17,10 - 17,30	Pharmacovigilance Meets Demographics: Towards Personalized Cardiotoxicity Prediction	Mateusz Iwan	Mario Negri Institute for Pharmacological Research IRCCS - Laboratory of Chemistry and Environmental Toxicology, Milan, Italy
17,30 - 17,50	From Data to Discovery: Streamlining QSAR Modeling and Molecular Docking with PoseidonQ and MzDOCK	Nicola Gambacorta	Università degli studi "Aldo Moro", Bari, Italy
19,30	**Social dinner - El Brellin**		

THURSDAY - 5 June 2025

TIME	SCHEDULE	PRESENTER	AFFILIATION
	(Q)SARs for screening, prioritization and data gap filling ***Section chairs: Uko Maran & Eva Bay Wedebye***		
9,00 - 9,20	Development of a structural alert profiler supporting the identification and characterisation of molecular initiating events associated with potential mechanisms of action for endocrine disruption	James W. Firman	Liverpool John Moores University, Liverpool, UK
9,20 - 9,40	QSAR-ME Profiler 2025, a new software for screening target chemicals and metabolites supported by similarity analysis and domain inspection	Ester Papa	University of Insubria, Varese, Italy
9,40 - 10,00	QSAR models for DIO1, DIO2 and DIO3 inhibition in the H2020 ATHENA project	Ana Caroline Vasconcelos Engedal Nissen	Technical University of Denmark, National Food Institute, Denmark
10,00 - 10,20	Custom QSAR Models for Assessing Azo Dye Genotoxicity	Prachi Pradeep	German Federal Institute for Risk Assessment (BfR), Berlin, Germany
10,20 - 10,40	Structural Alerts and Binary QSARs for the Prediction of Hepatic Steatosis	Anish Gomatam	Liverpool John Moores University, Liverpool, UK
10,40 - 11,20	***Coffee Break***		
11,20 - 11,50	KEYNOTE LECTURE OECD and the QSAR Toolbox: opening minds through meetings and guidance documents	Patience Browne	OECD, Paris, France
	In silico NAMs for regulatory purposes: industry perspective ***Section chairs: Nora Aptula & Mojca Fuart-Gatnik***		
11,50 - 12,10	Advancing Computational Toxicology: Consensus Machine Learning Models for Predicting Developmental and Reproductive Toxicity	Leonardo Contreas	Unilever, Sharnbrook, UK
12,10 - 12,30	Integration of in silico strategy for chemical screening and regulatory decision-making: finding the right compromise between automation and expert evaluation	Simona Kovarich	Merck Life Science, Milan, Italy
12,30 - 12,50	Can QSAR methods fully replace acute oral toxicity testing for EU REACH? Evaluation of the CATMoS Model	Anastasia Weyrich	BASF SE, Ludwigshafen, Germany
12,50 - 14,00	***Lunch***		
	In silico NAMs for regulatory purposes: regulators perspective ***Section chairs: Patience Browne & Andrea Gissi***		
14,00 - 14,20	Establishing Trust in Predicting Species Sensitivity Distributions for Chemical Risk Assessment	Pim N.H. Wassenaar	RIVM, Bilthoven, the Netherlands
14,20 - 14,40	The (Q)SAR Assessment Framework application at the European Chemicals Agency	Doris Hirmann	ECHA, Helsinki, Finland
14,40 - 15,45	Use of QSARs in regulatory frameworks: open questions and round table discussion	Andrea Gissi	EFSA, Parma, Italy
15,45 - 16,45	***Coffee break & POSTER SESSION***		
18,00	**Social activity - The impossible society**		

FRIDAY - 6 June 2025

TIME	SCHEDULE	PRESENTER	AFFILIATION
8,30 - 9,00	***Welcome Coffee***		
	Read-across, grouping, consensus modelling, and WoE ***Section chairs: Costanza Rovida & James Firman***		
9,00 - 9,20	Clustering of compounds with activities towards nuclear (endocrine) receptors considering different types of descriptors	Marjan Vračko	Kemijeki inštitut, Hajdrihova 10, 1000 Ljubljana, Slovenia
9,20 - 9,40	Advancing Regulatory Compliance with NAMs: A Read-Across Case Study for Mixture to Address Short-Term Repeated Dose Toxicity	Katarzyna Przybylak	Unilever, Safety, Environmental and Regulatory Science (SERS),Colworth Science Park, Sharnbrook, Bedford, UK
9,40 - 10,00	FlexFilters: A Modular Platform for Mining and Applying Structural Toxicity Alerts in Read-Across and QSAR Workflows	Suman Chakravarti	Multicase Inc., USA
10,00 - 10,20	Read-Across Applications: Lessons, Insights, and Best Practices	Arianna Bassan	Innovatune Srl, Padova, Italy
10,20 - 10,40	Confidently bridging the gap: A framework for decision support during read across	David Ponting	Lhasa Limited, Leeds, UK
10,40-11.,00	New consensus implementation of Cramer classification within the OECD QSAR Toolbox	Ksenia Gerova	Laboratory of Mathematical Chemistry, Burgas State University "Prof. D-r Assen Zlatarov", Burgas, Bulgaria
11,00 - 11,30	***Coffee Break***		
	In silico approaches for ecotox, green chemistry, sustainability and climate change ***Section chairs: Kunal Roy & Alessandro Sangion***		
11,30 - 12,00	The multiclass ARKA framework towards developing improved q RASAR models for environmental toxicity endpoints	Arkaprava Banerjee	Drug Theoretics and Cheminformatics Laboratory, Department of Pharmaceutical Technology, Jadavpur University, Kolkata 700 032, India
12,00 - 12,20	Ecological Risk Classification (ERC) strategy implemented in OECD QSAR Toolbox	Irina Dermen (Tsvetkova)	Laboratory of Mathematical Chemistry, Burgas State University "Prof. D-r Assen Zlatarov", Burgas, Bulgaria
12,20 - 12,40	Evaluation of PPCPs in Wastewater Treatment Plants: Combining QSAR Modeling with Monitoring data	Arianna Sgariboldi	QSAR Research Unit in Environmental Chemistry and Ecotoxicology, Department of Theoretical and Applied Sciences, University of Insubria, Varese, Italy. Department of Science and High Technology, University of Insubria, Como, Italy.
12,40 - 13,00	A new expert-based system to classify plant protection products according to their Mode of action	Anna Lombardo	Mario Negri Institute for Pharmacological Research IRCCS - Laboratory of Chemistry and Environmental Toxicology, Milan, Italy
13,00 - 13,20	Closing remarks & prize awards		
13,20 - 15,00	***Lunch & POSTER SESSION and end of the meeting***		