Alessandro Sangion

Alessandro.sangion@mail.utoronto.ca

About

Date of Birth: 12 Jun 1991 Citizenship: Italian, Swiss Cell. +1 416 527 1064

Language

Italian (Native speaker) English (C1, TOEFL iBT Score 103/120, Feb-2017) French (Basic level)

Scientific Interest

Bioaccumulation, Biotransformation, Chemical Hazard assessment Ecotoxicology Alternative to animal testing

Expertise

QSAR modelling, Multivariate analysis, Molecolar descriptors Chemometrics, Ecotoxicology

Technical Skill

Regression, Classification, Machine learning, Clustering, Data Curation, Database Management

Programming

R, advanced SQL, intermediate Python, beginner

Software

QSARINS,Knime, MySQLworkbench, Dragon, CDK, EPISuite, QSARToolbox, Statistica, ACDLab, Hyperchem, Office Package

In Brief

I am a MITACs Post-Doctoral Fellow at the University of Toronto Scarborough with Professor Frank Wania and Dr. Jon Arnot from ARC Inc. I have been working in the modelling field since 2013; I am experienced in QSAR model development and validation and in computational screening for environmental properties of organic chemicals

Current Position

Mitacs Elevate Postdoctoral Fellow

Since 02.2019
Toronto, Canada

University of Toronto Scarborough Academic Supervisor: Prof. Frank Wania

Partner Organization: Arnot Research and Consulting Inc, Dr Jon Arnot

- Project: A mass balance modelling framework for chemicals and their primary metabolites for ecological and human health assessment

Previous Position

Research Fellows

10.2018 - 01.2019

University of Insubria Varese, Italy

Scientific Supervisor: Prof. Ester Papa

Project: Database implementation, data analysis and QSAR modelling of biotransformation related endpoints in mammals in support of CEFIC LRI ECO44 Project iBAT-Mam Main Duties:

- Development, application and integration of QSAR models and related predictions in a framework for the estimation of bioaccumulation in mammals.
- Preparation of scientific manuscripts, reports and material for conferences.

Supervision of Master students.

Research Fellow

01.2014 - 06.2015

University of Insubria

Varese, Italy

Scientific Supervisor: Prof. Paola Gramatica

Project: Development of QSAR models for the environmental hazard estimation of emerging pollutants

Main Duties:

- Development, validation and application of QSAR models for the study of persistency, bioaccumulation and toxicity of pharmaceuticals and personal care products.
- Preparation of scientific manuscripts and material for conferences

Education

PhD in Chemistry and Environmental Sciences

10.2015 - 09.2018

University of Insubria

Varese, Italy

Supervisor: Prof. Ester Papa

Co-supervisor: Prof. Paola Gramatica

Project: QSAR models for the screening, prediction and refinement of PBT properties of Contaminants of Emerging Concern.

The general objective of the project is to apply QSAR methodologies to integrate biotransformation potential in the bioaccumulation assessment to refine PBT screening of organic contaminants.

Final Dissertation: 18 Gen 2019

International Visiting Graduate Student

05 - 08.2017

University of Toronto Scarborough

Toronto, Canada

Supervisors: Prof. Frank Wania, Adj Prof. Jon Arnot

Reference

Prof. Ester Papa University of Insubria Varese, Italy

ester.papa@uninsubria.it

Senior Prof. Paola Gramatica University of Insubria Varese, Italy paola.gramatica@uninsubria.it

Prof. Frank Wania University of Toronto Toronto, Canada

frank.wania@utoronto.ca

Adj Prof. Jon Arnot University of Torono Arnot Research and Consulting Inc.

Toronto, Canada

jon@arnotresearch.com

Project: Develop and apply methods to screen organic chemicals for their bioaccumulation potential in air-breathing organisms

This experience allowed me to get familiar with environmental fate and exposure models and enlarge my background about environmental modelling.

Guest PhD student 03 - 07.2016

Université Paris Diderot (Paris 7)

"Laboratoire ITODYS", UMR7086

Project.1: develop QSAR models for biotransformation potential in human Project.2: develop QSAR models for the cytotoxity of heterogenous nanoparticles

M.Sc in Environmental Sciences

09.2013 - 09.2015

Paris, France

University of Insubria

Varese, Italy

Final grade: 110/110 cum laude Supervisor: Prof. Paola Gramatica

Thesis: *Identification of environmental potential harmful Pharmaceuticals by QSAR modelling* The project was focused on the development and application of QSAR models to investigate the Persistence, Bioaccumulation and Toxic potential of Pharmaceuticals as environmental contaminants.

B.Sc in Natural and Environmental Sciences

09.2010 - 09. 2013

University of Insubria

Varese, Italy

Final grade: 110/110 cum laude Supervisor: Prof. Paola Gramatica

Award

Mitacs Elevate Postdoctoral Fellowship

2018

University of Toronto Scarborough Toronto, Canada

Academic Supervisor: Prof. Frank Wania

Partner Organization: Arnot Research and Consulting Inc

Project: A mass balance modelling framework for chemicals and their primary metabolites

for ecological and human health assessment

Conference Attendance Grants

2014

XXV Congresso Nazionale della Società Chimica Italiana

Arcavacata di Rende, Italy

Contribution presented: Poster

Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS"

Teaching

Teacher assistant

Winter Session 2018-2019

University of Insubria

Varese, Italy

Course: Chemical methodologies for the environment part1: Applied Environmental Chemistry

Tenured professor: Prof. Ester Papa

Tasks: Frontal lessons and student supervision during the computational laboratory of chemometric.

Teacher assistant

Winter Session 2017-2018

University of Insubria

Varese, Italy

Course: Chemical methodologies for the environment part1: Applied Environmental Chemistry

Tenured professor: Prof. Ester Papa

Tasks: Frontal lessons and student supervision during the computational laboratory of chemometric.

Teacher assistant

Winter Session 2016-2017

University of Insubria

Varese, Italy

Course: Chemical methodologies for the environment part1: Applied Environmental Chemistry Tenured professor: Prof. Paola Gramatica

Tasks: Frontal lessons and student supervision during the computational laboratory of chemometric.

Teacher assistant

Winter Session 2015-2016

University of Insubria Varese, Italy

Course: Chemometric and Ecotoxicological test: Chemometric

Tenured professor: Prof. Paola Gramatica

Tasks: Frontal lessons and student supervision during the computational laboratory of

chemometric.

Other Activities

Supervisor of undergraduate students

Since 2017

At University of Insubria

Varese, Italy

- Ilaria Casartelli

- Linda bertato
- Daniele Scarabelli
- Lucrezia Motta

At University of Toronto

Toronto, Canada

- Moosa Said

Reviewer for International Scientific Journals

Since 2017

- Science of Total Environment
- Chemosphere
- Journal of Chemometrics

Students' representative for the Chemistry and Environmental Sciences doctoral school at Department of Science and High Technology (DiSAT), University of Insubria, Varese, Italy from 2016 to 2018

Reference: Prof. Norberto Masciocchi

Co-Author, beta- tester and users assistant for the software for QSAR Multiple Linear

Regression models development and validation "QSARINS" since 2013

Reference: Prof. Paola Gramatica

Volunteer in the natural park "PLIS Valle Lanza" in Malnate, Italy since 2013 Tasks: Guide in organized guided tour, front desk in conference and festivals

Reference: Dr. Marco Pizzato

Publications

13. Gramatica Paola, Papa Ester, Sangion Alessandro

"QSAR Modeling of Cumulative Environmental End-Points for the Prioritization of Hazardous Chemicals"

Environmental Science: Processes & Impacts, 2018, 20 (1): 38–47. doi.org/10.1039/C7EM00519A

12. Papa Ester, Sangion Alessandro, Arnot Jon A, Gramatica Gramatica

"Development of Human Biotransformation QSARs and Application for PBT Assessment Refinement"

Food and Chemical Toxicology, 2018, 112(2): 535-43. doi.org/10.1016/J.FCT.2017.04.016

11. Papa Ester, <u>Sangion Alessandro</u>, Taboureau Olivier, Gramatica Paola "Quantitative Prediction of Rat Hepatotoxicity by Molecular Structure"

International Journal of Quantitative Structure-Property Relationships, 2018, 3 (2): 12

10. Papa Ester, Arnot Jon A., Sangion Alessandro, Gramatica Paola

"In Silico Approaches for the Prediction of In Vivo Biotransformation Rates" In Advances in QSAR Modeling, 2017, 425–51. Springer

doi.org/10.1007/978-3-319-56850-8_11

9. Caruso Enrico, Gariboldi Marzia, <u>Sangion Alessandro</u>, Gramatica Paola, Banfi Stefano "Synthesis, Photodynamic Activity, and Quantitative Structure-Activity Relationship Modelling of a Series of BODIPYs"

Journal of Photochemistry and Photobiology B: Biology, 2017, 167: 269–81. doi.org/10.1016/J.JPHOTOBIOL.2017.01.012

8. Sangion Alessandro, Gramatica Paola

"Ecotoxicity Interspecies QAAR Models from Daphnia Toxicity of Pharmaceuticals and Personal Care Products"

SAR and QSAR in Environmental Research, 2016, 27 (10): 781–98 doi.org/10.1080/1062936X.2016.1233139

7. Sangion Alessandro, Gramatica Paola

"Hazard of Pharmaceuticals for Aquatic Environment: Prioritization by Structural Approaches and Prediction of Ecotoxicity"

Environment International, 2016, 95(10): 131-43. doi.org/10.1016/J.ENVINT.2016.08.008

6. Sangion Alessandro, Gramatica Paola

"PBT Assessment and Prioritization of Contaminants of Emerging Concern: Pharmaceuticals" *Environmental Research*, 2016, 147(5): 297–306. doi.org/10.1016/J.ENVRES.2016.02.021

5. Papa Ester, Doucet Jean Pier, Sangion Alessandro, Doucet-Panaye Annick

"Investigation of the Influence of Protein Corona Composition on Gold Nanoparticle Bioactivity Using Machine Learning Approaches"

SAR and QSAR in Environmental Research, 2016, 27 (7): 521–38.

doi.org/10.1080/1062936X.2016.1197310

4. Gramatica Paola, Sangion Alessandro

"A Historical Excursus on the Statistical Validation Parameters for QSAR Models: A Clarification Concerning Metrics and Terminology"

Journal of Chemical Information and Modeling, 2016, 56 (6): 1127–31. doi.org/10.1021/acs.jcim.6b00088.

3. Gramatica Paola, Cassani Stefano, Sangion Alessandro

"Aquatic Ecotoxicity of Personal Care Products: QSAR Models and Ranking for Prioritization and Safer Alternatives' Design."

Green Chemistry, 2016, 18 (16): 4393–4406. doi.org/10.1039/C5GC02818C SELECTED AS COVER PAGE

2. Gramatica Paola, Cassani Stefano, Sangion Alessandro

"Are Some 'Safer Alternatives' Hazardous as PBTs? The Case Study of New Flame Retardants" Journal of Hazardous Materials, 2016, 306 (5): 237–46. doi.org/10.1016/J.JHAZMAT.2015.12.017.

1. Gramatica Paola, Cassani Stefano, Sangion Alessandro

"PBT Assessment and Prioritization by PBT Index and Consensus Modeling: Comparison of Screening Results from Structural Models."

Environment International, 2015, 77 (4): 25–34. doi.org/10.1016/J.ENVINT.2014.12.012

Seminars

Sangion Alessandro

"Biotransformation QSARs & software demonstration"

In: Training Course: The Application of Emerging Tools for Bioaccumulation Assessment: Integration of Biotransformation; Sponsored by CEFIC-LRI and Health and Environmental Sciences Institute (HESI)

Platforms

11. Sangion Alessandro, Arnot Jon A., Gramatica Paola, Papa Ester.

"QSAR models for the screening, prediction and refinement of PBT Properties of Contaminants of Emerging Concern"

Platform presentation in: Merck – Elsevier Young Chemist Symposium 2018, Rimini, Italy

- 10. Sangion Alessandro, Arnot Jon A., Gramatica Paola, Papa Ester.
- "A Tiered Approach for Screening Chemicals for Biomagnification Potential in Humans" Platform presetation in: 6th Chemoinformatics Strasbourg Summer School. 2018, Strasbourg, France
- 9. Sangion Alessandro, Arnot Jon A., Gramatica Paola, Papa Ester.
- "A Tiered Approach for Screening Chemicals for Biomagnification Potential in Humans" Platform presetation in: 18th International Conference on QSAR in Environmental and Health Sciences, 2018. Bled, Slovenia
- 8. Sangion Alessandro, Arnot Jon A., Gramatica Paola, Papa Ester.
- "A Tiered Approach for Screening Chemicals for Biomagnification Potential in Humans" Platform presetation in: SETAC Europe 28th annual meeting, 2018. Rome, Italy
- 7. <u>Sangion Alessandro</u>, Papa Ester, Arnot Jon A., Gramatica Paola. Platform presentation in: Merck Young Chemists Symposium XVII edition, 2017. Milano Marittima, Italy.
- 6. <u>Sangion Alessandro</u>, Papa Ester, Arnot Jon A., Gramatica Paola. Platform presentation in: 6th Young Environmental Scientists Meeting (SETAC YES). 2017. Stockholm, Sweden.
- 5. Papa Ester, Sangion Alessandro

"Quantitative Structure-Activity Relationships to predict the cytotoxicity of heterogeneous nanoparticles"

Platform presentation in: SCI XVI Congresso Nazionale della Divisione di Chimica dell'Ambiente e dei Beni Culturali, 2016. Lecce, Italy

- 4. Sangion Alessandro, Cassani Stefano, Papa Ester, Gramatica Paola
- "Screening and prioritization of chemicals for PBT behavior: state of the art on the consensus approach by PBT Index and PBT Profiler"

Platform presentation in: SETAC Europe 26th annual meeting, 2016. Nantes, France

- 3. Sangion Alessandro, Cassani Stefano, Papa Ester, Gramatica Paola
- "Identification of potential environmentally hazardous pharmaceuticals by QSAR modeling" Platform presentation in: Workshop of SETAC Italian Branch: "Monitoring and control of priority micro-pollutants in water and removal techniques in plants treating water for human consumption and in waste water" in Ecomondo, the Green technologies expo, 2015. Rimini, Italy
- 2. <u>Sangion Alessandro</u>, Cassani Stefano, Papa Eser, Gramatica Paola "Identification of potential environmentally hazardous pharmaceuticals by QSAR modeling" Platform presentation in: SCI XV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, 2015. Bergamo, Italy.
- 1. <u>Sangion Alessandro</u>, Cassani Stefano, Papa Eser, Gramatica Paola "Identification of potential environmentally hazardous pharmaceuticals by QSAR modeling" Platform presentation in: SETAC Europe 25th annual meeting, 2015. Barcelona, Spain

Posters

20. Foster Karen L., Looky Alexandra B, Armitage James B, Embry Michelle, <u>Sangion Alessandro</u>, Papa Ester, Arnot Jon A.

"A Human in Vitro Biotransformation Rate Database for QSAR model development" In: 18th International Conference on QSAR in Environmental and Health Sciences, 2018. Bled, Slovenia

19. Sangion Alessandro, Gramatica Paola

"QSAR Studies on the Potential Environmental Hazard of Pharmaceuticals"

In: 1st International Conference on Risk Assessment of Pharmaceuticals in the Environment (ICRAPHE), 2016. Paris, France

18. Papa Ester, Sangion Alessandro, Gramatica Paola

"Prediction and screening of the human biotransformation half-lives of heterogeneous substances by in silico approaches"

In: SCI XVI Congresso Nazionale della Divisione di Chimica dell'Ambiente e dei Beni Culturali, 2016. Lecce, Italy

17. Sangion Alessandro, Gramatica Paola, Papa Ester

"L'approccio QSAR nella Green Chemistry: modelli computazionali per lo studio della tossicità e l'impatto ambientale di farmaci"

In: 4° Workshop Nazionale Gruppo Interdivisionale Green Chemistry-Chimica Sostenibile 2016. Firenze, Italy, SELECTED AS POSTER SPOTLIGHT

16. Sangion Alessandro, Gramatica Paola

"QSAR Studies on the Potential Environmental Hazard of Pharmaceuticals"

In: SETAC Europe 26th annual meeting, 2016. Nantes, France

15. Sangion Alessandro, Gramatica Paola, Cassani Stefano.

"Are some "safer alternatives" of Flame Retardants hazardous as PBTs? Screening of FRs by the cumulative PBT Index in QSARINS"

In: SETAC Europe 26th annual meeting, 2016. Nantes, France

14. Papa Ester, Sangion Alessandro, Gramatica Paola

"QSAR prediction of human Biotransformation Half-Lives: models development and application"

In: SETAC Europe 26th annual meeting, 2016. Nantes, France

13. Sangion Alessandro, Cassani Stefano, Gramatica Paola,

"Pharmaceuticals ecotoxicity: data curation and QSAR modeling"

In: Workshop of SETAC Italian Branch: "Monitoring and control of priority micro-pollutants in water and removal techniques in plants treating water for human consumption and in waste water" in Ecomondo, the Green technologies expo, 2015. Rimini, Italy

12. Cassani Stefano, Sangion Alessandro, Marzetta Francois, Gramatica Paola

"PBT assessment of Personal Care Products"

In: Workshop of SETAC Italian Branch: "Monitoring and control of priority micro-pollutants in water and removal techniques in plants treating water for human consumption and in waste water" in Ecomondo, the Green technologies expo, 2015. Rimini, Italy

11. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Interspecies QAAR for pharmaceuticals"

In: SCI XV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, 2015. Bergamo, Italy.

10. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Pharmaceuticals ecotoxicity: data curation and QSAR modeling"

In: SCI XV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, 2015. Bergamo, Italy.

9. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Interspecies QAAR for pharmaceuticals"

In: SETAC Europe 25th annual meeting, 2015. Barcelona, Spain

8. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Pharmaceuticals ecotoxicity: data curation and QSAR modeling"

In: SETAC Europe 25th annual meeting, 2015. Barcelona, Spain

7. Gramatica Paola, Sangion Alessandro, Cassani Strefano

"Come disegnare composti piu' sicuri: l'approccio "Benign by Design

In: Planet Green Chem, il primo congresso della chimica verde, sostenibile e innovativa, 2015. Milano, Italy.

6. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS"

In: XXV Congresso Nazionale della Società Chimica Italiana, 2014. Arcavacata di Rende, Italy

5. Cassani Stefano, Sangion Alessandro, Gramatica Paola

"How to avoid dangerous alternative to banned chemicals in a benign by design approach: screening of Flame Retardants by the cumulative PBT-Index in QSARINS"

In: XXV Congresso Nazionale della Società Chimica Italiana, 2014. Arcavacata di Rende, Italy

4. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS"

In: 16th International Workshop on Quantitative Structure-Activity Relationship in Environmental and Health Sciences, 2014. Milano, Italy

3. Cassani Stefano, Sangion Alessandro, Gramatica Paola

"How to avoid dangerous alternative to banned chemicals in a benign by design approach: screening of Flame Retardants by the cumulative PBT-Index in QSARINS"

In: 16th International Workshop on Quantitative Structure-Activity Relationship in Environmental and Health Sciences, 2014. Milano, Italy

2. Cassani Stefano, Sangion Alessandro, Gramatica Paola

"How to avoid dangerous alternative to banned chemicals in a benign by design approach: screening of Flame Retardants by the cumulative PBT-Index in QSARINS"

In: SETAC Europe 24th annual meeting, 2014. Basel, Switzerland

1. Sangion Alessandro, Cassani Stefano, Gramatica Paola

"Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS"

In: SETAC Europe 24th annual meeting, 2014. Basel, Switzerland. SELECTED AS POSTER SPOTLIGHT

Platforms and Poster presented by other authors

In: 18th International Conference on QSAR in Environmental and Health Sciences, 2018. Bled, Slovenia

- Invited Opening Presentation: "Chemometric QSAR modelling for hazard assessment and priority setting", <u>P. Gramatica</u>, E. Papa, **A. Sangion**.
- Platform Presentation: "QSAR prediction of biotransformation half-lives and application for PBT assessment refinement", <u>E. Papa</u>, **A. Sangion**, J. Arnot, P. Gramatica.
- Poster: "The new QSARINS-Chem", P. Gramatica, A. Sangion, N. Chirico, E. Papa.
- Poster: "QSAR-like approaches to address nanoparticles activity: lights and shades", <u>E. Papa</u>, J.P. Doucet, A. Doucet-Panaye, **A. Sangion**, M. Hemadi.
- Poster: "Prediction of the triplet-sensitized phototransformation of phenols induced by chromophoric dissolved organic matter by QSAR models", <u>E. Papa</u>, L. Motta, **A. Sangion**, P. Gramatica, M. Minella, D. Vione.

In: SETAC Europe 28th annual meeting, 2018. Rome, Italy.

- Platform Presentation: "Development of biotransformation half-life QSARs and PBT assessment refinement of Pharmaceuticals and Personal Care Products", <u>E. Papa</u>, **A. Sangion**, J. Arnot, P. Gramatica.

- Poster: "In Silico approaches for the screening and the design of safer chemicals", <u>E. Papa</u>, **A. Sangion**, P. Gramatica.
- Poster: "QSAR: a predictive approach for electronic cigarettes toxicological assessment", <u>D. Zarini</u>, E. Papa, **A. Sangion**, E. Caruso, S. Zucchi, S. Sterpone, E. Ferri.
- Poster: "In silico investigation of the triplet-sensitised phototransformation of phenols induced by chromophoric dissolved organic matter", E. Papa, <u>L. Motta</u>, **A. Sangion**, P. Gramatica, M. Minella, D. Vione.

In: 19th International Symposium on Environmental Pollution and its Impact on Life in the Mediterranean Region (MESAEP), 2017. Rome, Italy

Poster: "Molecular Structure and Computational QSAR Models can help in identifying Hazardous Chemicals and in designing more environmentally sustainable compounds", P. Gramatica, E. Papa, A. Sangion.

16th International Conference On Chemistry And The Environment (ICCE), 2017. Oslo, Norway

- Platform Presentation: "Benign by design approach for more sustainable chemicals: QSAR modeling for the prioritization of chemicals of environmental concern", <u>P.</u> Gramatica, **A. Sangion**, E. Papa.
- Poster: "Potential environmental hazard of emerging pollutants: QSAR models in the new version of the QSARINS software", P. Gramatica, A. Sangion, E. Papa.
- Poster: "Prediction of in vivo biotransformation in fish and human for the refinement of bioaccumulation", E. Papa, A. Sangion, J. Arnot, T. Brown, L. van der Wal, <u>P. Gramatica</u>
 In: SETAC Europe 27th annual meeting, 2017. Brussels, Belgium.
 - Platform Presentation: "Nonlinear learning systems for predicting nanoparticle toxicity",
 N. Toschi, S. Ciulli, S. Diciotti, E. Papa, A. Sangion, A. Duggento, M. Guerrisi, A. Magrini,
 L. Campagnolo, A. Pietroiusti.
 - Poster: "Prediction of in vivo biotransformation in fish and human for the refinement of bioaccumulation", **E. Papa**, A. Sangion, J. Arnot, T. Brown, L. van der Wal, P. Gramatica.
 - Poster: "Quantitative relationships between the structure of pharmaceuticals and the expression of genes involved in liver damage", E. Papa, S. Abbar, M. Petitjean, A. Sangion, O. Tabureau.
 - Poster: "In silico approaches for the prediction of the cytotoxic activity of heterogeneous nanoparticles", **E. Papa**, A. Sangion, S. Diciotti, S. Ciulli, A. Duggento, M. Guerrisi, A. Magrini, L. Campagnolo, A. Pietroiusti, N. Toschi.

In: Last International Meeting of the COST Action TD1204 MODENA 2016. Zagreb, Croatia

- Invited Presentation: "QSAR Models for heterogeneous Nanoparticles Results from the COST Action D1204 MODENA - WG3 Exercise", E. Papa, A. Sangion

In: 6th EuCheMS Chemistry Congress, 2016. Seville, Spain

 Selected Poster Spotlight: "Molecular Structure and Computational Models Can Help in Identifying Hazardous Chemicals and in Designing More Environmentally Sustainable Compounds", P. Gramatica, A. Sangion, E. Papa.

In: SCI XVI Congresso Nazionale della Divisione di Chimica dell'Ambiente e dei Beni Culturali, 2016. Lecce, Italy

- Poster: "QSAR modeling of the PBT behaviour and the Aquatic Toxicity Index of PPCPs", P. Gramatica, A. Sangion, S. Cassani, E. Papa.

In: 17th International Conference on QSAR in Environmental and Health Sciences, 2016. Miami Beach, USA

- Platform Presentation: "QSAR modeling of the PBT behaviour and the Aquatic Toxicity Index of PPCPs", <u>P. Gramatica</u>, **A. Sangion**, S. Cassani.
- Selected Poster Spotlight: "QSARINS-Chem: a database of environmental chemicals and QSAR models", P. Gramatica, S. Cassani, N. Chirico, A. Sangion.
- Poster: "QSAR Studies on the Environmental Hazard of Pharmaceuticals", **A. Sangion**, S. Cassani, <u>P. Gramatica</u>.

- Poster: "QSAR Modeling and prioritization of Personal Care Products", S. Cassani, A. Sangion, P. Gramatica.

In: SETAC Europe 26th annual meeting, 2016. Nantes, France

 Poster: "PBT Behavior and Aquatic Ecotoxicity of Personal Care Products: QSAR modeling and prioritization", <u>P. Gramatica</u>, S. Cassani, **A. Sangion**

In: 18th International Symposium on Environmental Pollution and its Impact on Life in the Mediterranean Region (MESAEP), 2015. Crete, Greece.

- Platform Presentation: "Screening and Prioritization of Chemicals for REACH: the Cumulative PBT Index Model in QSARINS", <u>P. Gramatica</u>, S. Cassani, **A. Sangion**, E. Papa.
- Poster: "How to draw safest chemicals: the benign by design approach", <u>P. Gramatica</u>, **A. Sangion**, S. Cassani. Poster.

In: 15th EuCheMS International Conference on Chemistry and the Environment (ICCE), 2015. Leipzig, Germany.

- Platform Presentation: "Screening and Prioritization of Chemicals for REACH: the Cumulative PBT Index Model in QSARINS", P. Gramatica, A. Sangion, S. Cassani, E. Papa.
- Poster: "How to avoid dangerous alternative to banned chemicals in a safer approach: screening of Flame Retardants by the cumulative PBT Index in QSARINS", <u>P. Gramatica</u>, **A. Sangion**, S. Cassani.
- Poster: "Pharmaceuticals ecotoxicity: data curation and QSAR modeling", <u>P. Gramatica</u>, **A. Sangion**, S. Cassani.
- Poster: "QSARINS: software for the development, analysis and validation of MLR models and QSARINS-Chem: insubria datasets and QSA(P)R models for environmental pollutants", P. Gramatica, **A. Sangion**, S. Cassani, N. Chirico.

In: 51st Congress of the European Societies of Toxicology (EUROTOX),2015. Porto, Portugal

- Poster: "Screening and Prioritization of Chemicals for REACH: the Cumulative PBT Index Model in QSARINS", P. Gramatica, S. Cassani, A. Sangion, E. Papa.
- Poster: "Pharmaceutical Ecotoxicity: Data Curation and QSAR Modeling", <u>P. Gramatica</u>, **A. Sangion**, S. Cassani.

In: Conferentia Chemometrica, 2015. Budapest, Hungary.

- Platform Presentation: "Screening and Prioritization of chemicals for REACH: modeling of Persistence, Bioaccumulation and Toxicity by the PBT Index", <u>S. Cassani</u>, **A. Sangion**, E. Papa, P. Gramatica.
- Poster: "Interspecies QAAR for pharmaceuticals", A. Sangion, S. Cassani, P. Gramatica.
- Poster: "How to avoid dangerous alternative to banned chemicals in a safer approach: screening of Flame Retardants by the cumulative PBT Index in QSARINS", <u>S. Cassani</u>, **A. Sangion**, P. Gramatica.
- Poster: "QSARINS: software for the development, analysis and validation of MLR models and QSARINS-Chem: Insubria dataset and QSAR models for environmental pollutants", S. Cassani, N. Chirico, A. Sangion, P. Gramatica.

In: 8th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI), 2015. Chios, Greece.

- Platform Presentation: "Screening and prioritization of chemicals for REACH: the cumulative PBT index model in QSARINS", P. Gramatica, S. Cassani, A. Sangion, E. Papa.
- Poster: "Pharmaceuticals ecotoxicity: data curation and QSAR modeling", P. Gramatica, A. Sangion, S. Cassani.
- Poster: "QSARINS: software for the development, analysis and validation of MLR models and QSARINS-Chem: Insubria datasets and QSA(P)R models for environmental pollutants", P. Gramatica, N. Chirico, A. Sangion, S. Cassani.

In: SCI, XV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, 2015. Bergamo, Italy

- Platform Presentation: "QSAR Modeling and further priority setting of Personal Care Products", S. Cassani, **A. Sangion**, F. Marzetta, P. Gramatica.
- Poster: "PBT assessment of Personal Care Products", <u>S. Cassani</u>, **A. Sangion**, F. Marzetta, P. Gramatica.
- Poster: "Prediction and screening of fish biotransformation half-lives", <u>E. Papa</u>, L. van der
 Wal, J. Arnot, **A. Sangion**, S. Cassani, P. Gramatica.

In: SETAC Europe 25th annual meeting, 2015. Barcelona, Spain

- Platform Presentation: "QSAR Modeling and further priority setting of Personal Care Products", <u>S. Cassani</u>, **A. Sangion**, F. Marzetta, P. Gramatica.
- Selected Poster Spotlight: "Prediction and screening of fish biotransformation half-lives".
 E. Papa, L. van der Wal, J. Arnot, A. Sangion, S. Cassani, P. Gramatica.
- Poster: "PBT assessment of Personal Care Products", <u>S. Cassani</u>, **A. Sangion**, F. Marzetta, P. Gramatica.

In: SETAC North America 35th Annual Meeting, 2014. Vancouver, Canada.

- Platform Presentation: "From Chemical Structure to Environmental Hazard: exploiting QSAR for screening, prioritization and safer alternative design", P. Gramatica, S. Cassani, S. Kovarich, N. Chirico, A. Sangion, L. Ceriani, E. Papa. Platform Presentation.
- Poster: "QSARINS: software for development, analysis, validation of MLR models; QSARINS-Chem: Insubria datasets and QSA(P)R models for environmental pollutants", <u>P. Gramatica</u>, N. Chirico, S. Kovarich, S. Cassani, E.Papa, **A. Sangion**.
- Poster: "How to avoid dangerous alternative to banned chemicals in benign by design approach: screening of Flame Retardants by cumulative PBT Index in QSARINS", <u>P. Gramatica</u>, S. Cassani, **A. Sangion**.
- Poster: "Screening and prioritization of Perfluorinated Chemicals and Personal Care Products in QSARINS-Chem", <u>P. Gramatica</u>, N. Chirico, **A. Sangion**, S. Cassani.

In: XXV Congresso Nazionale della Società Chimica Italiana, 2014. Arcavacata di Rende, Italy

- Keynote Presentation: "From Chemical structure to environmental hazard: Exploiting QSAR for screening, prioritization and safer alternative design". P. Gramatica, S. Cassani, S. Kovarich, N. Chirico, A. Sangion, E. Papa.
- Platform Presentaion: "QSARINS: new software for development and validation of MLR models; QSARINS-Chem: datasets and QSAR models for environmental pollutants", <u>S.</u> Cassani, N. Chirico, E. Papa, S. Kovarich, **A. Sangion**, P. Gramatica.
- Poster: "Priority setting of PFCs and Personal Care Products in QSARINS-Chem", <u>S. Cassani</u>, N. Chirico, **A. Sangion**, A. Fracasso, P. Gramatica.

In: 16th International Workshop on Quantitative Structure-Activity Relationship in Environmental and Health Sciences, 2014. Milano, Italy

- Platform Presentation: "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", <u>S. Cassani</u>, N. Chirico, E. Papa, S. Kovarich, **A. Sangion**, P. Gramatica.
- Poster: "Screening and prioritization of Perfluorinated Chemicals and Personal Care Products in QSARINS-Chem", <u>S. Cassani</u>, N. Chirico, <u>A. Sangion</u>, A. Fracasso, P. Gramatica.
 In: 10th International Conference on Chemical Structures (ICCS), 2014. Noordwijkerhout, The Netherland.
- Poster: "QSARINS: software for the development, analysis and validation of MLR models, and QSARINS-Chem: Insubria datasets and QSA(P)R models for environmental pollutants". P. Gramatica, N. Chirico, A. Sangion, S. Cassani.