General information about QSARINS

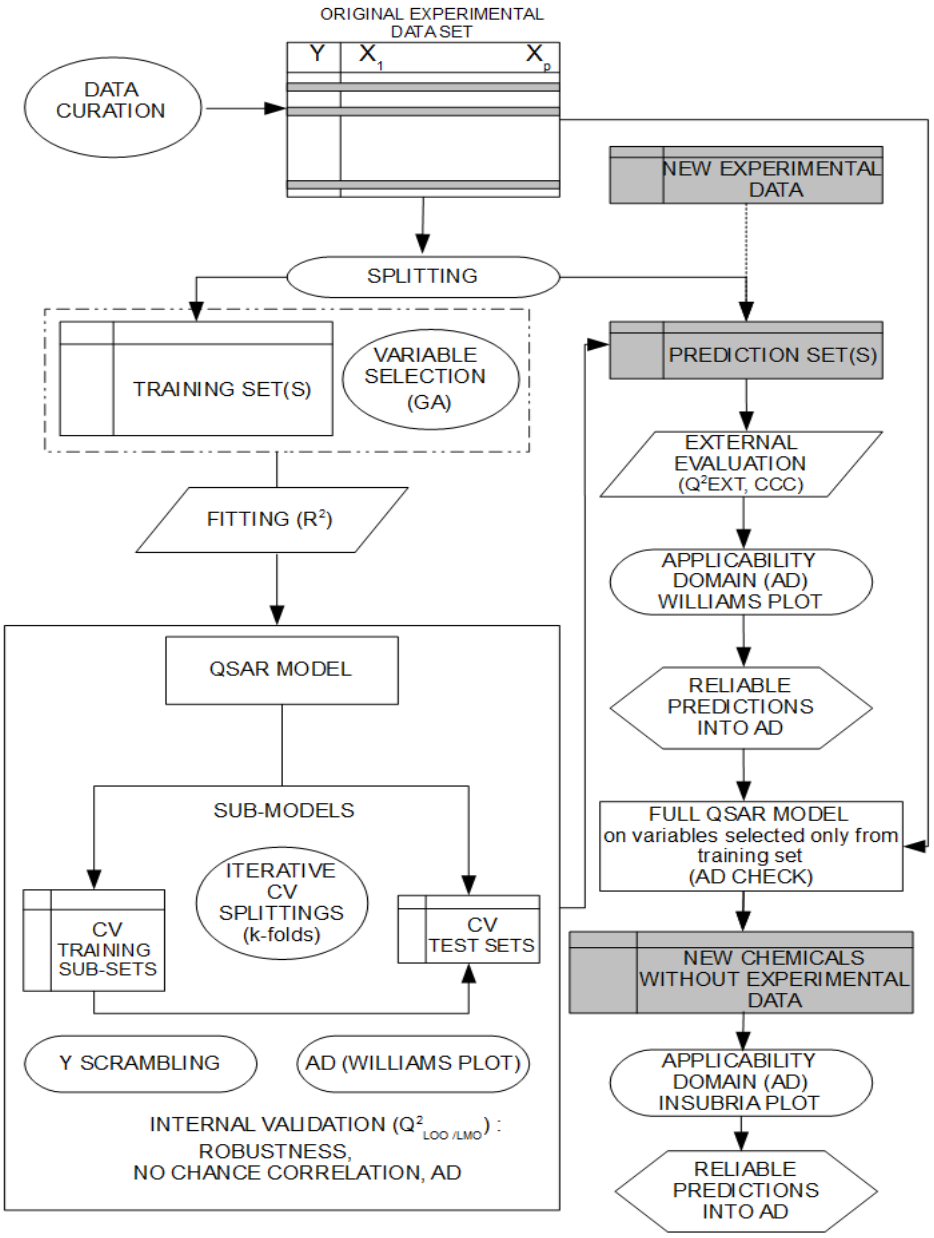
QSARINS (QSAR INSubria) is a software for the development and validation of Multiple Linear Regression (MLR) models by Ordinary Least Squares (OLS), developed by Nicola Chirico (2008-2014) and implemented according to the statistical approach for predictivity [Gramatica, 2007, 2009, 2012, 2014], which is applied by the QSAR group of the University of Insubria. The software is presented in the following paper:

Gramatica, P., Chirico, N., Papa, E., Kovarich, S., Cassani, S. QSARINS: A New Software for the Development, Analysis, and Validation of QSAR MLR Models. *Journal of Computational Chemistry*, *Software news and updates*, **2013**, 34, 2121-2132, DOI: 10.1002/jcc.23361.

The new version of QSARINS, including the new module "QSARINS-Chem", is presented in the following paper:

Gramatica, P., Cassani, S., Chirico, N. QSARINS-Chem: Insubria Datasets and New QSAR/QSPR Models for Environmental Pollutants in QSARINS. *Journal of Computational Chemistry*, *Software news and updates*, **2014**, 35, 1036-1044, DOI: 10.1002/jcc.23576.

The following Scheme summarizes the procedure:



QSARINS is mainly focused on external validation of MLR QSAR models, according to the underline philosophy explained in two fundamental papers by Prof. Gramatica [Gramatica 2007, 2014].

QSARINS provides a user-friendly interface that includes tools for:

- Data normalization;

- Dataset analysis (by Principal Component Analysis, etc.);

- Splitting of the data sets (by Random, Sorted response or Structure);

- OLS Model development by All Subset Selection;

- Genetic Algorithm (GA) for Variable Selection (with tracing of the models while being developed);

- Analysis of all individual variables, as well as those more frequently selected in the models;

- Internal validation, including the following criteria: Q^2_{LOO}, Q^2_{LMO}, RMSE, MAE, Y-Scrambling, etc…;

- External validation, including the following criteria: Q^2_{F1}, Q^2_{F2}, Q^2_{F3}, Golbraikh and Tropsha parameters, r^2_m metrics, Concordance Correlation Coefficient (CCC);

- Determination of the structural Applicability Domain by the leverage from the diagonal values of the Hat matrix (including the Williams graph for chemicals with experimental data, y axis: standardized residuals and and Insubria graph for those without data, y axis: predicted values);

- Multi-Criteria Decision Making (MCDM);

- Combined modeling (weighted and not, different tools for selection of models);

- Check and validation of imported single models;

- Principal Components (PC) Regression;

- PBT Index model [Papa and Gramatica, 2010];

- Application of several QSAR/QSPR models developed using PaDEL-Descriptor 2.18 [Yap, 2011] and stored in QSARINS, with the relative QMRF (QSAR Model Reporting Format);

- Ranking chemicals, based on PCA and MCDM;

- Database of compounds used to develop Insubria QSAR models; chemicals can be explored in different ways (**CAS**, **SMILES**, **names**) and visualized in 3D;

- Calculation of molecular descriptors and fingerprints with the open source software PaDEL-Descriptor.

All outcomes of QSARINS are reported in the software with corresponding **plots** for quick graphical interpretation.

Additional information

QSARINS can be used for every modeling work involving Multiple Linear Regression (MLR) calculations, based on Genetic Algorithm for variable selection and Ordinary Least Squares (OLS) as modelling method. Other chemometric tools (Principal Component Analysis (PCA), Multicriteria Decision Macking (MCDM)) for

explorative analysis and ranking are also implemented, thus it is not limited to Quantitative Structure-Activity Relationships (QSAR) studies. The objects studied in QSAR modeling are chemicals, but they could be any kind of objects in other modeling studies.

QSARINS-Chem is the module where 2828 chemicals, studied by the Insubria group, are available with their 3D structure and experimental responses. In addition, 23 QSAR models of environmental end-points, based on free software for molecular descriptors (PaDEL-Descriptor 2.18) are available. These models, supported by their QMRF, can be applied for any new chemical.

It is important to note that any user can upload personal data sets and models and use QSARINS to manage them for storing, visualization, modeling, ranking etc.

Citation and acknowledgements

In any publication, derived from the use of QSARINS software, this must be cited as:

Gramatica, P., Chirico, N., Papa, E., Cassani, S., Kovarich, S., QSARINS: A New Software for the Development, Analysis, and Validation of QSAR MLR Models. Journal of Computational Chemistry, Software news and updates, **2013**, 34, 2121-2132, DOI: 10.1002/jcc.23361.

and

Gramatica, P., Cassani, S., Chirico, N. QSARINS-Chem: Insubria Datasets and New QSAR/QSPR Models for Environmental Pollutants in QSARINS. *Journal of Computational Chemistry*, *Software news and updates*, **2014**, 35, 1036-1044, DOI: 10.1002/jcc.23576.

and the provider should be acknowledged and the website www.qsar.it should be cited.

References:

Paola Gramatica, 2007. Principles of QSAR models validation: internal and external
QSAR Comb.Sci. 26(5), 694-701

Paola Gramatica, 2009. Chemometric Methods and Theoretical Molecular Descriptors in Predictive QSAR Modeling of the Environmental Behaviour of Organic Pollutants, Chapter 12 in *Recent Advances in QSAR Studies ,* Tomasz Puzyn - Jerzy Leszczynski - Mark T.D. Cronin Eds., (Challenges and Advances in Computational Chemistry and Physics), Springer-Verlag New York Inc, Nov. pp. 327-366.

Paola Gramatica, 2012. Modeling Chemicals in the Environment. Chap. 17 in *Drug Design Strategies-Quantitative Approaches,* D.J.Livingstone and A.M.Davies Eds., RSC Pub., pp. 458-478.

Yap Chun Wei, 2011. PaDEL-Descriptor: An open source software to calculate molecular descriptors and fingerprints. *J.Comput. Chem. 32 (7), 1466-1474*

Paola Gramatica, 2014. External Evaluation of QSAR Models, in Addition to Cross-Validation: Verification of Predictive Capability on Totally New Chemicals. Mol. Inf. 33, 311-314.

QSARINS is currently used by the Insubria group and some other groups, and has been used and cited in the following publications and scientific contributions:

Nicola Chirico and Paola Gramatica (2011)
Real External Predictivity of QSAR Models: How To Evaluate It? Comparison of Different Validation Criteria and Proposal of Using the Concordance Correlation Coefficient.
J. Chem. Inf. Model. 51 (9), pp 2320–2335. DOI: 10.1021/ci200211n

Nicola Chirico and Paola Gramatica (2012)
Real External Predictivity of QSAR Models. Part 2. New inter-comparable thresholds for different validation criteria and the need for scatter plot inspection.
J. Chem. Inf. Model 52 (8), pp 2044–2058. DOI: 10.1021/ci300084j

Paola Gramatica, Stefano Cassani, Partha Pratim Roy, Simona Kovarich, Yap Chun Wei, and Ester Papa (2012)
QSAR modeling is not “push a button and find a correlation”: a case study of acute toxicity of (benzo-)triazoles on algae.
Mol.Inf. 31, pp 817-835. DOI: 10.1002/minf.201200075

Stefano Cassani, Simona Kovarich, Ester Papa, Partha Pratim Roy, Leon van der Wal, and Paola Gramatica (2013)
Daphnia and fish toxicity of (benzo)triazoles: validated QSAR models, and interspecies quantitative activity-activity modelling.
J.Hazard Mat. 258-259, pp 50-60. DOI: 10.1016/j.jhazmat.2013.04.025

Stefano Cassani, Simona Kovarich, Ester Papa, Partha Pratim Roy, Magnus Rahmber2, Sara Nilsson, Ullrika Sahlin, Nina Jeliazkova, Nikolay Kochev, Ognyan Pukalov, Igor V. Tetko, Stefan Brandmaier, Mojca Kos Durjava, Boris Kolar, Willie Peijnenburg and Paola Gramatica (2013)
Evaluation of CADASTER QSAR models for aquatic toxicity of (benzo-)triazoles and prioritization by consensus.
ATLA 41, pp 49-64.

Paola Gramatica (2013)
On the Development and Validation of QSAR Models.
Chap. 21 in Computational Toxicology: Volume II, Methods in Molecular Biology, vol. 930, Brad Reisfeld and Arthur N. Mayeno (eds.), 2012, DOI 10.1007/978-1-62703-059-5_21, Springer Science+Business Media, LLC, N.Y. (USA), 2013, pp 499-526.

Vikas, Reenu, Chayawan(2013)
Does electron-correlation has any role in the quantitative structure–activity relationships?
J.Mol.Graph. Model. 42, pp 7-16. DOI: 10.1016/j.jmgm.2013.02.005.

Ester Papa, Simona Kovarich, and Paola Gramatica (2013)
QSAR prediction of the competitive interaction of emerging halogenated pollutants with human transthyretin
SAR QSAR Environ. Res. 24 (4), pp 599-615. DOI:10.1080/1062936X.2013.773374

Jiazhong Li, Huanxiang Liu, Xing Huo, Paola Gramatica (2013)
Structure-Activity Relationship Analysis of the Thermal Stabilities of Nitroaromatic Compounds Following Different Decomposition Mechanisms.
Mol.Inf. 32, pp 193-202. DOI: 10.1002/minf.201200089

Jiazhong Li, Shuyan Li, Chongliang Bai, Huanxiang Liu, Paola Gramatica (2013)
Structural requirements of 3-carboxyl-4(1H)-quinolones as potential antimalarials from 2D and 3D QSAR analysis
J. Mol. Graphics Modell. 44, pp 266-277. DOI: 10.1016/j.jmgm.2013.07.004

Simona Funar-Timofei, Sorin Avram, Ana Borota (2013)
Structure-Toxicity Study of Some Pyrethroidal Esters Insecticides.
Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, Vol. 17, e012; doi:10.3390/ecsoc-17-e012, http://www.sciforum.net/conference/ecsoc-17/paper/2250

Simona Funar-Timofei, Liliana Halip, Ana Borota, Alina Bora (2013)
Quantitative Structure-Activity Study of Some Cyclin-Dependent Kinase 5/P25 Inhibitors
Timisoara's Academic Days, XIIIth Edition. New Trends and Strategies in the Chemistry of Advanced materials with relevance in Biological Systems, technique and Environmental Protection, 13-14 June 2013, Timisoara, Romania, ISSN: 2065-0760, p. 46, Poster.

Reenu, Vikas (2014)
Electron-correlation based externally predictive QSARs for mutagenicity of nitrated-PAHs in Salmonella typhimurium TA100
Ecotox. Environ. Safe., 101, pp. 42-50. DOI: 10.1016/j.ecoenv.2013.11.020

Vijay H. Masand, Devidas T. Mahajan, Taibi Ben Hadda, Rahul D. Jawarkar, Hemant Chavan, B. P. Bandgar, Harsh Chauhan (2014)
Molecular Docking and Quantitative Structure Activity Relationship (QSAR) Analyses Of Indolylarylsulfones As HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors
*Med. Chem. Re*s. 23, pp 417-425. DOI: 10.1007/s00044-013-0647-8

Ester Papa, Leon van der Wal, John. A. Arnot, and Paola Gramatica (2014)
Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis
Sci. Total Environ. 470-471, pp 1040-1046. DOI: 10.1016/j.scitotenv.2013.10.068.

Vijay H. Masand, Devidas T. Mahajan, Taibi Ben Hadda, Rahul D. Jawarkar, Ahmed M. Alafeefy, Vesna Rastija, Mohamed Ashraf Ali (2014)
Does tautomerism influence the outcome of QSAR modeling?
*Med. Chem. Re*s. 23, pp 1742-1757. DOI: 10.1007/s00044-013-0776-0

Vesna Rastija, Vijay H. Masand (2014)
QSAR of Antitrypanosomal Activities of Polyphenols and their Analogues Using Multiple Linear Regression and Artificial Neural Networks
Comb. Chem. High Throughput Screen. 17(8), pp 709-717. DOI:
10.2174/13862073176661408041616O5

Yonghua Shao, Jining Liu, Meixia Wang, Lili Shi, Xiaojun Yao, Paola Gramatica (2014)
Integrated QSPR models to predict the soil sorption coefficient for a large diverse set of compounds by using different modeling methods
Atmos. Environ. 88, pp 212-218. DOI: 10.1016/j.atmosenv.2013.12.018.

Vikas, Chayawan (2014)
Externally predictive quantitative modeling of supercooled liquid vapor pressure of polychlorinated-naphthalenes through electron-correlation based quantum-mechanical descriptors
Chemosphere 95, pp 448-454. DOI: 10.1016/j.chemosphere.2013.09.093.

Rajni Garg and Carr J. Smith (2014)
Predicting the bioconcentration factor of highly hydrophobic organic chemicals
Food Chem. Toxicol. 69, pp 252-259. DOI: http://dx.doi.org/10.1016/j.fct.2014.03.035

Paola Gramatica (2014)
External Evaluation of QSAR models, in Addition to Cross-Validation: Verification of Predictive Capability of Totally New Chemicals
Mol. Inf. 33, pp 311-314. DOI: 10.1002/minf.201400030

Vijay H. Masand, Andrey A. Toropov, Alla P. Toropova, Devidas T. Mahajan (2014)
QSAR Models for Anti-Malarial Activity of 4-Aminoquinolines
Curr. Comput. Aided Drug Des. 10, pp 75-82. DOI: 10.1002/minf.201400030

Takahiro Suzuki, Sorin Avram, Ana Borota, Simona Funar-Timofei (2014)
QSAR Modeling of N3-Substituted Imidacloprid Insecticides Used Against the Housefly *Musca Domestica*
Journal of Tokyo University, Natural Science, 58, pp 83-95 (ISSN: 0372-0330)

Suvendu Biswas, Roger Kayaleh, Girinath G. Pillai, Christopher Seon, Ian Roberts,
Vadim Popov, Khalid A. Alamry, and Alan R. Katritzky (2014)
Long-Range Chemical Ligation from N->N Acyl Migrations in Tryptophan Peptides via Cyclic Transition States of 10- to 18-Members
Chem. Eur. J., 20, pp 1 – 11. DOI: 10.1002/chem.201400125

Rok Martinčič, Katja Venko, Špela Župerl, Marjana Novič (2014)
Chemometrics approach for the prediction of structure–activity relationship for membrane transporter bilitranslocase
SAR QSAR Environ. Res. 25, pp 853-872. DOI: 10.1080/1062936X.2014.962082

Gulcin Tugcu, Birkan Yilmaz, Melek Türker Saçan (2014)
Comparative performance of descriptors in a Multiple Linear and Kriging Models: A case study on the acute toxicity of organic chemicals to algae
Environ. Sci. Pollut. Res. DOI: 10.1007/s11356-014-3182-3. Poster presented at ICCE 2013, Barcelona, Spain. 25-28 June 2013.

Syed Nasir Abbas Bukhari, Ibrahim Jantan, Vijay H. Masand, Devidas T. Mahajan, Muhammad Sher, M. Naeem-ul-Hassan, Muhammad Wahab Amjad (2014)
Synthesis of a, b-unsaturated carbonyl based compounds as acetylcholinesterase and butyrylcholinesterase inhibitors: Characterization, molecular modeling, QSAR studies and effect against amyloid b-induced cytotoxicity
Eur. J. Med. Chem. 83, pp 355-365. DOI: 10.1016/j.ejmech.2014.06.034

Luana Janaína de Campos, Eduardo Borges de Melo (2014)
Modeling structure–activity relationships of prodiginines withantimalarial activity using GA/MLR and OPS/PLS
J. Mol. Graphics Modell. 54, pp 19-31. DOI: 10.1016/j.jmgm.2014.08.004

Lili Xi, Shuyan Li, Xiaojun Yao, Yuhui Wei, Jiazhong Li, Huanxiang Liu, Xin'an Wu (2014)
In Silico Study Combining Docking and QSAR Methods on a Series of Matrix Metalloproteinase 13 Inhibitors
Arch. Pharm. 347, pp 825–833. DOI: 10.1002/ardp.201400200

Vijay H. Masand, Devidas T. Mahajan, Paola Gramatica, James Barlow (2014)
Tautomerism and multiple modelling enhance the efficacy of QSAR: antimalarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl
Med. Chem. Res. 23, pp 4825-4835. DOI: 10.1007/s00044-014-1043-8

Simona Funar-Timofei, Smaranda Iliescu, Takahiro Suzuki (2014)
Correlations of limiting oxygen index with structural polyphosphoester features by QSPR approaches
Struct. Chem. 25, pp 1847-1863. DOI: 10.1007/s11224-014-0474-7

Enis Örücü, Gulcin Tugcu, Melek Türker Saçan (2014)
Molecular structure–adsorption study on current textile dyes
SAR QSAR Environ. Res. 25, pp 983-998. DOI: 10.1080/1062936X.2014.976266

Vijay H. Masand, Devidas T. Mahajan, Gulam M. Nazeruddin, Taibi Ben Hadda, Vesna Rastija, Ahmed M. Alfeefy (2015)
Effect of descriptor selection before splitting and method of splitting (rational and random) on external predictive ability and on behaviour of different statistical parameters of QSAR model
Med. Chem. Res. 24, pp 1241-1264. DOI: 10.1007/s00044-014-1193-8

U. Judycka-Proma, L. Bober, A.Gajewicz, T. Puzyn, J. Błażejowski (2015)
Chemometric analysis of correlations between electronic absorption characteristics and structural and/or physicochemical parameters for ampholytic substances of biological and pharmaceutical relevance
Spectrochim. Acta Mol. Biomol. Spectros. 138, pp 700-710. DOI: 10.1016/j.saa.2014.11.067

Paola Gramatica, Stefano Cassani, Alessandro Sangion (2015)
PBT Assessment and prioritization by PBT Index and consensus modeling: Comparison of screening results from structural models
Environ. Int. 77, pp 25-34. DOI: 10.1016/j.envint.2014.12.012

Vikas, Chayawan (2015)
Single-descriptor based quantum-chemical QSPRs for physico-chemical properties of polychlorinated-dibenzo-p-dioxins and -dibenzo-furans (PCDD/Fs): Exploring the role of electron-correlation
Chemosphere 118, pp 239-245. DOI: 10.1016/j.chemosphere.2014.08.072

Eslam Pourbasheer, Reza Aalizadeh, Jamal Saffar Ardabili, Mohammad Reza Ganjali (2015)
QSPR study on solubility of some fullerenes derivatives using the genetic algorithms — Multiple linear regression
J. Mol. Liq. 204, pp 162-169. DOI:10.1016/j.molliq.2015.01.028

Rok Martinčič, Igor Kuzmanovski, Alain Wagner, Marjana Novič (2015)
Development of models for prediction of the antioxidant activity of derivatives of natural compounds
Anal. Chim. Acta 868, pp 23-35. DOI:10.1016/j.aca.2015.01.050

Lidia Ceriani, Ester Papa, Simona Kovarich, Robert Boethling, Paola Gramatica (2015)
Modeling ready biodegradability of fragrance materials
Environ. Toxicol. Chem. 34, pp 1224-1231. DOI: 10.1002/etc.2926

Alicja Mikolajczyk, Agnieszka Gajewicz, Bakhtiyor Rasulev, Nicole Schaeublin, Elisabeth Maurer-Gardner, Saber M. Hussain ,Jerzy Leszczynski, Tomasz Puzyn (2015)
Zeta Potential (ζ) for Metal Oxide Nanoparticles: A Predictive Model Developed by Nano-QSPR Approach
Chem. Mater. 27, pp 2400-2407. DOI: 10.1021/cm504406a

Celina Sikorska (2015)
Toward predicting vertical detachment energies for superhalogen anions exclusively from 2-D structures
Chem. Phys. Lett. 625, pp 157-163. DOI: 10.1016/j.cplett.2015.03.002

Siva S. Panda, Rachel J. Jones, C. Dennis Hall, Alan R. Katritzky
Applications of Chemical Ligation in Peptide Synthesis via Acyl Transfer
Top. Curr. Chem. 362, pp 229-266. DOI: 10.1007/128_2014_608

Vikas, Reenu (2015)
Role of exchange and correlation in the real external prediction of mutagenicity: performance of hybrid and meta-hybrid exchange–correlation functionals
RSC Adv. 5, pp 29238–29251. DOI: 10.1039/c4ra14262d

Villu Ruusmann, Sulev Sild, Uko Maran (2015)
QSAR DataBank repository: open and linked qualitative and quantitative structure–activity relationship models
J. Cheminform. 7:32 pp 1-11. DOI: 10.1186/s13321-015-0082-6

Vijay H. Masand, Devidas T. Mahajan, Ahmed M. Alafeefy, Syed Nasir Abbas Bukhari, Nahed N. Elsayed (2015)
Optimization of antiproliferative activity of substituted phenyl 4-(2-oxoimidazolidin-1-yl) benzenesulfonates: QSAR and CoMFA analyses
Eur. J. Pharm. Sci. 77 pp 230-237. DOI: 10.1016/j.ejps.2015.06.001

Mihai V. Putz, Nicoleta A. Dudaș, Adriana Isvoran (2015)
Double Variational Binding—(SMILES) Conformational Analysis by Docking Mechanisms for Anti-HIV Pyrimidine Ligands
Int. J. Mol. Sci. 16 pp 19553-19601. DOI:10.3390/ijms160819553

María Jimena Martínez, Ignacio Ponzoni, Mónica F Díaz, Gustavo E Vazquez, Axel J Soto (2015)
Visual analytics in cheminformatics: user‐supervised descriptor selection for QSAR methods
J. Cheminform. 7:39 pp 1-17. DOI 10.1186/s13321-015-0092-4

Reza Aalizadeh, Eslam Pourbasheer, Mohammad Reza Ganjali (2015)
Analysis of B-Raf^{V600E} inhibitors using 2D and 3D-QSAR, molecular docking and pharmacophore studies
Mol. Divers. In press, accepted article. DOI 10.1007/s11030-015-9626-y

Jiazhong Li, Fang Bai, Huanxiang Liu, Paola Gramatica (2015)
Ligand Efficiency Outperforms pIC50 Both on 2D MLR and 3D CoMFA Models – A Case Study on AR Antagonists
Chem. Biol. Drug. Des. In press, accepted article. DOI: 10.1111/cbdd.12619

Saeed Yousefinejad, Bahram Hemmateenejad (2015)
Chemometrics tools in QSAR/QSPR studies: A historical perspective
Chemometr. Intell. Lab. In press, accepted manuscript. DOI:10.1016/j.chemolab.2015.06.016

Paola Gramatica, Stefano Cassani, Alessandro Sangion (2015)
Are Some "Safer Alternatives" hazardous? The Case Study of New Flame Retardants
Under revision on *J.Hazard Mater.*

Lucky Ahmed, Bakhtiyor Rasulev, Jerzy Leszczynski (2015)
Inhibitors or Toxins? Comprehensive Investigations of Interactions Between Fullerene Derivatives and Ample Set of Proteins
Submitted to *Nat. Nanotechnol.*

Paola Gramatica, Nicola Chirico, Stefano Cassani, Simona Kovarich, Ester Papa (2014)
QSARINS: a new software for the development, analysis and validation of MLR models and QSARINS-Chem: Insubria datasets and new QSAR/QSPR models for environmental pollutants.
Oral Platform at SETAC Europe 24th Annual Meeting, Basel (Switzerland), 11-15 May 2014.

Stefano Cassani, Paola Gramatica (2014)
How to focus experimental tests only on priority Personal Care Products.
Poster at SETAC Europe 24th Annual Meeting, Basel (Switzerland), 11-15 May 2014.

Stefano Cassani, Paola Gramatica (2014)
Screening and ranking of PFASs by MultiCriteria Decision Making approach in QSARINS for highlighting the priority compounds.
Poster at SETAC Europe 24th Annual Meeting, Basel (Switzerland), 11-15 May 2014.

Alessandro Sangion, Stefano Cassani, Paola Gramatica (2014)
Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS.
Poster spotlight at SETAC Europe 24th Annual Meeting, Basel (Switzerland), 11-15 May 2014.

Stefano Cassani, Alessandro Sangion, Paola Gramatica (2014)
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.
Poster at SETAC Europe 24th Annual Meeting, Basel (Switzerland), 11-15 May 2014.

Paola Gramatica, Nicola Chirico, Alessandro Sangion, Stefano Cassani (2014)
QSARINS: software for the development, analysis and validation of MLR models, and QSARINS-Chem: Insubria datasets and QSA(P)R models for environmental pollutants.
Poster at 10th International Conference on Chemical Structures, Noordwijkerhout (Netherlands), 1-5 June 2014.

Stefano Cassani, Nicola Chirico, Ester Papa, Simona Kovarich, Alessandro Sangion, Paola Gramatica (2014)
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.
Oral Platform at 16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014). Milan (Italy), 16-20 June 2014.

Stefano Cassani, Alessandro Sangion, Paola Gramatica (2014)
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.
Poster at 16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014). Milan (Italy), 16-20 June 2014.

Stefano Cassani, Nicola Chirico, Alessandro Sangion, Andrea Fracasso, Paola Gramatica (2014)
Screening and prioritization of Perfluorinated Chemicals and Personal Care Products in QSARINS-Chem.
Poster at 16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014). Milan (Italy), 16-20 June 2014.

Alessandro Sangion, Stefano Cassani, Nicola Chirico, Paola Gramatica (2014)
Screening and prioritization of chemicals in the context of REACH: the cumulative PBT Index model implemented in QSARINS software.
Poster at 16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014). Milan (Italy), 16-20 June 2014.

Stefano Cassani, Nicola Chirico, Ester Papa, Simona Kovarich, Alessandro Sangion, Paola Gramatica (2014)
QSARINS: new software for development and validation of MLR models; QSARINS-Chem: datasets and QSAR models for environmental pollutants.
Oral Platform at XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Rende (Italy), 7-12 September 2014

Paola Gramatica, Stefano Cassani, Simona Kovarich, Nicola Chirico, Alessandro Sangion, Ester Papa (2014)
From Chemical Structure to Environmental Hazard: exploiting QSAR for screening, prioritization and safer alternative design
Keynote lecture at XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Rende (Italy), 7-12 September 2014

Stefano Cassani, Francois Marzetta, Paola Gramatica (2015)
QSAR Modeling and further priority setting of Personal Care Products
Platform at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Stefano Cassani, Alessandro Sangion, Francois Marzetta, Paola Gramatica (2015)
PBT assessment of Personal Care Products
Poster at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Alessandro Sangion, Stefano Cassani, Ester Papa, Paola Gramatica (2015)
Identification of potential environmentally hazardous pharmaceuticals by QSAR modeling
Platform at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Alessandro Sangion, Stefano Cassani, Paola Gramatica (2015)
Interspecies QAAR for pharmaceuticals
Poster at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Alessandro Sangion, Stefano Cassani, Paola Gramatica (2015)
Pharmaceuticals ecotoxicity: data curation and QSAR modeling
Poster at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Ester Papa, Leon van der Wal, Jon Arnot, Alessandro Sangion, Stefano Cassani, Paola Gramatica (2015)
Prediction and screening of fish Biotransformation half-lives
Platform at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Ester Papa, Leon van der Wal, Jon Arnot, Paola Gramatica (2015)
Recent Advances in QSAR prediction of fish and human Biotransformation Half lives
Poster at SETAC Europe 25th Annual Meeting, Barcelona (Spain), 3-7 May 2015

Paola Gramatica, Alessandro Sangion, Stefano Cassani (2015)
Come disegnare composti più sicuri: l'approccio "benign by design"
Poster at Planet Green Chem, Primo Congresso della Chimica Verde, Sostenibile e Innovativa, Milano (Italy), 30 March – 1 April 2015

Stefano Cassani, Francois Marzetta, Paola Gramatica (2015)
QSAR Modeling and further priority setting of Personal Care Products
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