# *QSARINS*

***Software for QSAR MLR model development and validation***




## How to cite:

Each user of QSARINS (whether for QSAR models' development/validation or for application of QSARINS-Chem models or for use of the stored Insubria datasets) must cite the web: www.qsar.it and the following papers, where the software is presented:

- 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.
- 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

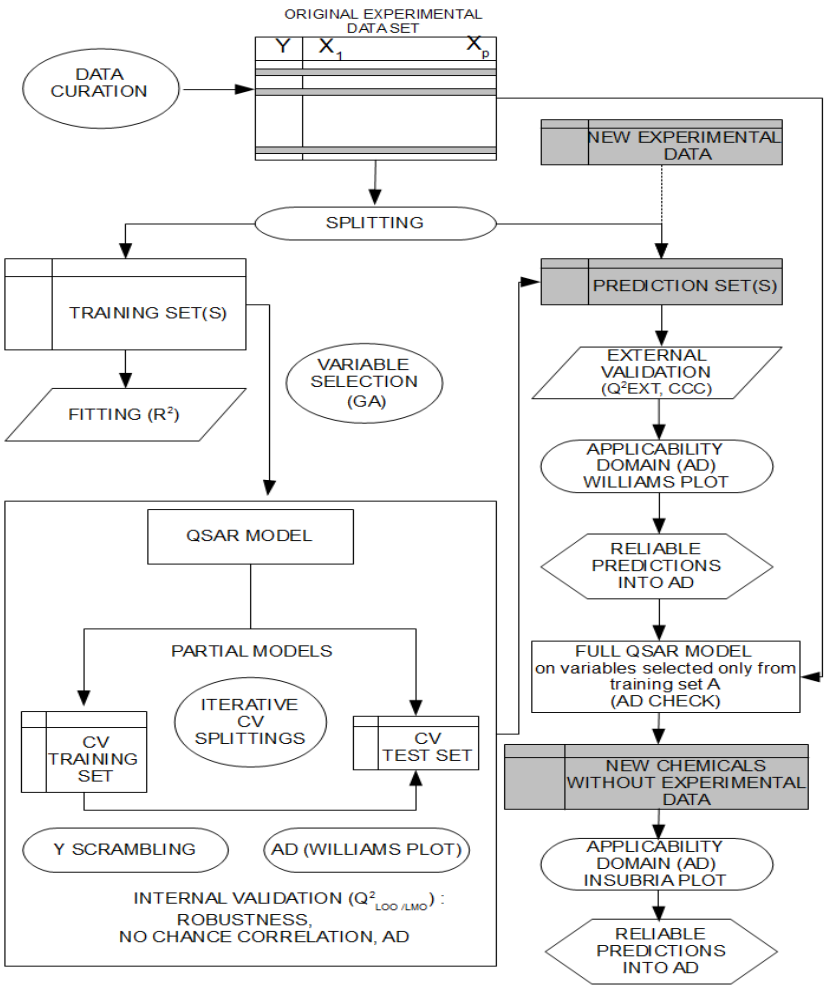
The provider Prof. Paola Gramatica should also be acknowledged for the free license.

## 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 (2008-2012) and implemented according to the statistical approach for QSAR models' predictivity (Tropsha et al. 2003; Gramatica 2007, 2009, 2012, 2013, 2014, 2016, Chirico and Gramatica 2011, 2012; Gramatica et al. 2012; Gramatica and Sangion 2016), which is applied by the QSAR group of the University of Insubria in all the modeling researches.

In the module **QSARINS-Chem** the 3D- chemical structures of the Insubria datasets are stored, in addition to several QSAR models, based on PaDEL Descriptors, developed by the Insubria QSAR group and applicable also to new chemicals, directly in QSARINS, where the PaDEL Descriptors can be calculated.

The following scheme (from Gramatica et al. *Mol. Inf.* 2012) summarizes the procedure for a validated QSAR modeling, applicable in QSARINS:



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

- Data normalization;

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

- Splitting of the data sets (by Random, Ordered response or Structure by PCA of molecular descriptors);

- 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: $Q^2_{LOO}$, $Q^2_{LMO,}$ Concordance Correlation Coefficient (CCC), 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, $CCC_{EXT}$, RMSE, MAE;

- Structural applicability domain by the leverage from the diagonal values of the Hat matrix (including Williams plot for chemicals with experimental data, y axis: standardized residuals and Insubria graph for chemicals without data, y axis: predicted values);

- Principal Components (PCs) Regression;

- Multi-Criteria Decision Making (MCDM) for selection of the best models;

- Consensus modeling (weighted and not, different tools for selection of models to be average);

- Check and validation of imported single models;

-Calculation of molecular descriptors and fingerprints with the open source software PaDEL-Descriptor [Yap, 2011] (version currently included: 2.21).

- Application of several QSAR/QSPR models for environmental pollutants, developed by PaDEL-Descriptor software and stored in the QSARINS-Chem module, with the corresponding QMRF (QSAR Model Reporting Format). In particular:

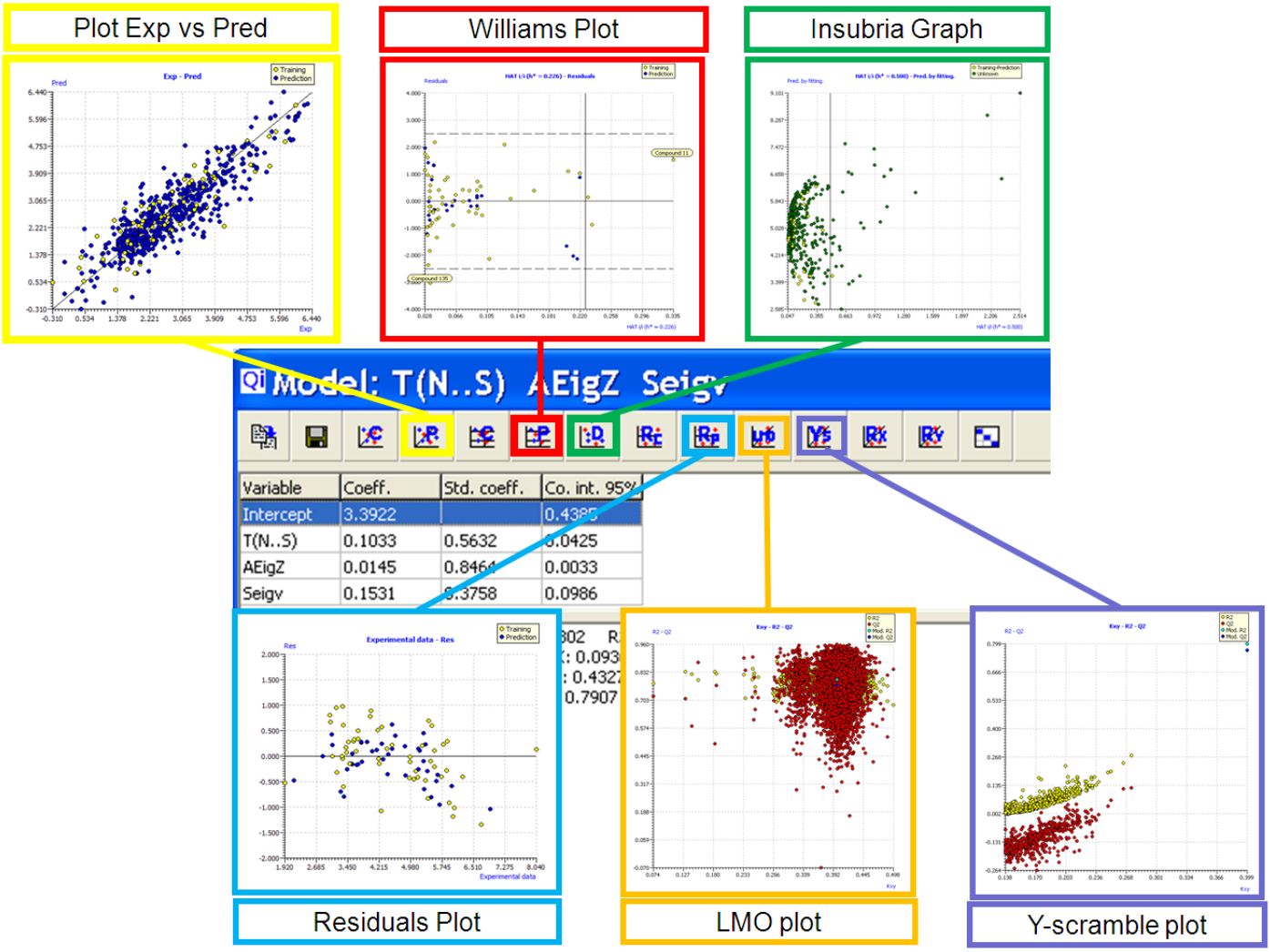
- PBT Index model [Papa and Gramatica, 2010], re-developed using PaDEL-Descriptor [Yap, 2011];

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

- Ranking of chemicals, based on PCA and MCDM;

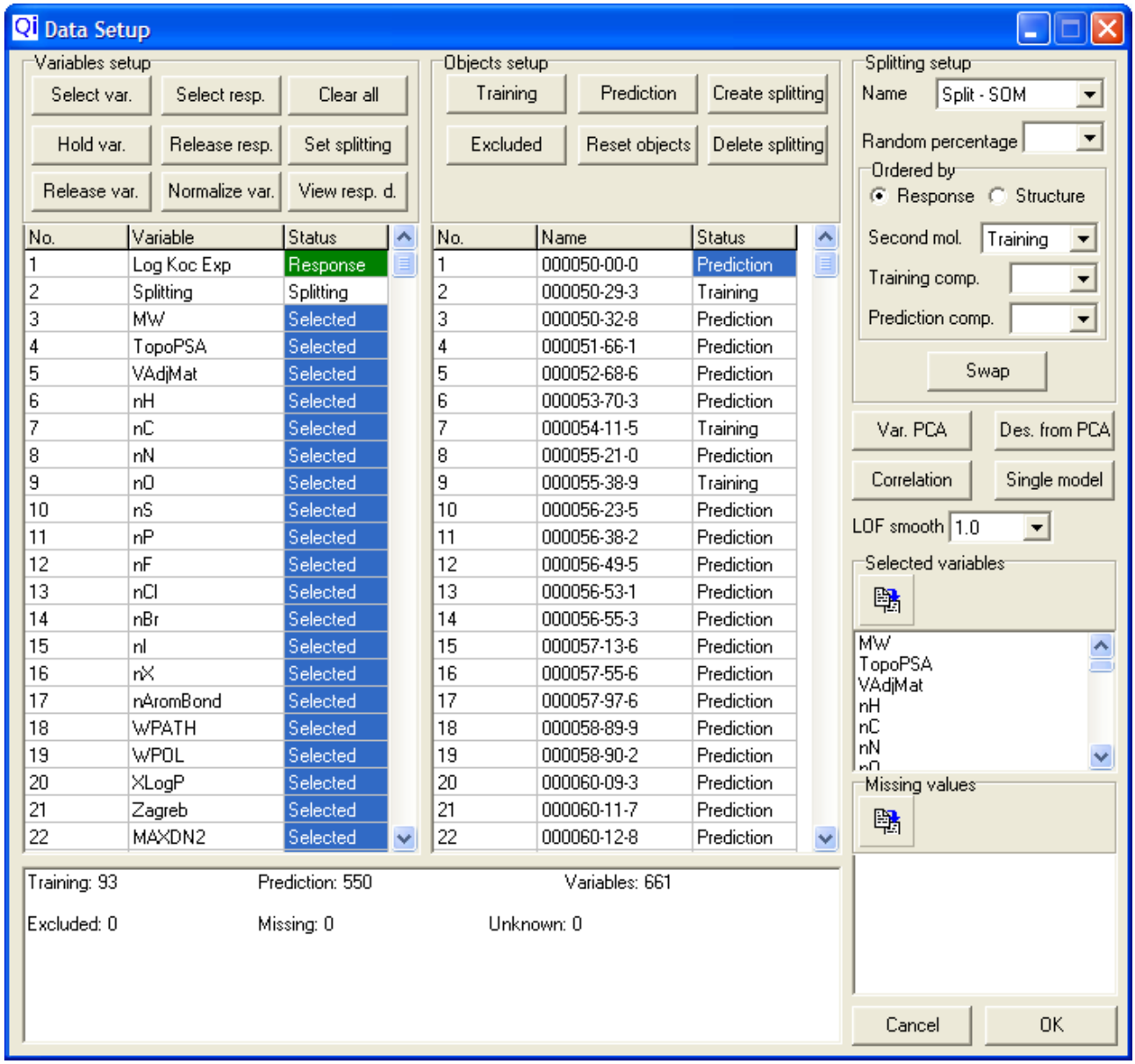
All outcomes of QSARINS are reported in the software with corresponding **plots** for quick graphical interpretation.

Example of some available **plots:**



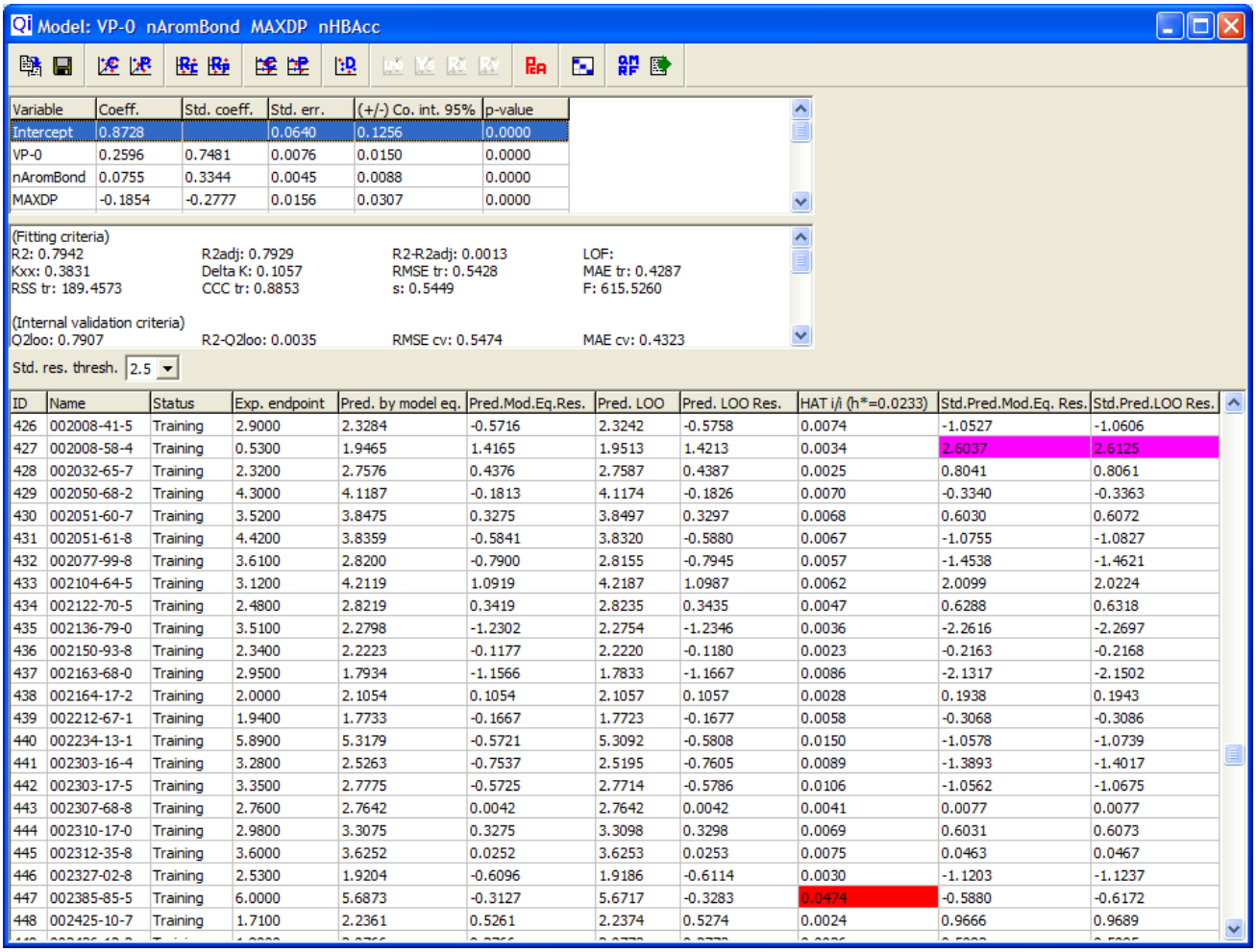
**SCREENSHOTS**

**DATA SETUP** - Selection of variables and response. Three different splitting (Random, by ordered response, by structure based on PCA of molecular descriptors). PCA of the selected descriptors and generation of PC scores as variables for Principal Components Regression.



**SINGLE MODEL** – Model's parameters related to internal and external validation, predicted values, HAT values, and standardized residuals are calculated.
In addition, it is possible to view the PCA and the correlation matrix of the modeling descriptors. If available, the QMRF can be exported. It is present for the large majority of the models available in QSARINS-Chem.

**IMPORTANT INFORMATION: Any user can upload personal MLR models and use QSARINS to manage them for storing, visualization, validation, ranking etc..**



## QSARINS-Chem

QSARINS-Chem is the module where 3014 chemicals, collected from the literature, curated and modeled by the Insubria group, are available with their 3D structure and experimental responses. In addition, 40 QSAR models of environmental end-points for organic pollutants, based on free software for molecular descriptors (PaDEL-Descriptor 2.18/2.21 by Yap Chun Wei, presented in: PaDEL-Descriptor: An open source software to calculate molecular descriptors and fingerprints. *J.Comput. Chem.* 2011, 32 (7), 1466-1474), are available. These models, supported by their QMRF, can be applied for any new chemical without experimental data or also not yet synthesized, verifying the structural applicability domain by the Insubria graph.

## List of QSAR models in QSARINS-Chem:

1. Brominated Flame Retardants (BFR) Log Koa (Papa et al. 2009)
2. BFR MP (Papa et al. 2009)
3. BFR VP (Papa et al. 2009)
4. Benzo-Triazole (BTAZ) *D. magna* tox (Cassani et al. 2013)
5. BTAZ Log Kow (Bhhatarai and Gramatica 2011a)
6. BTAZ MP (Bhhatarai and Gramatica 2011a)
7. BTAZ *O. mykiss* tox (Cassani et al. 2013)
8. BTAZ *P. subcapitata* tox (Cassani et al. 2013)
9. BTAZ Sw (Bhhatarai and Gramatica 2011a)
10. BTAZ VP (Bhhatarai and Gramatica 2011a)
11. Endocrine Disruptor Chemicals (EDC) Estrogen Receptor Binding (Li and Gramatica 2010)
12. Esters *D. magna* tox (Papa et al. 2005a)
13. *Esters P. promelas* tox (Papa et al. 2005a)
14. Fish Biotrans. logHLn M1_day (Papa et al. 2014)
15. Fish Biotrans. logHLn M2_day (Papa et al. 2014)
16. Fish Biotrans. logHLn M3_day (Papa et al. 2014)
17. Global Half-Life Index (GHLI) (Gramatica and Papa 2007)
18. Human Biotrans. logHLB1_h (Papa et al. 2018)
19. Human Biotrans. logHLB2_h (Papa et al. 2018)
20. Human Biotrans. logHLB3_h (Papa et al. 2018)
21. Human Biotrans. logHLB4_h (Papa et al. 2018)
22. Human Biotrans. logHLT_h (Papa et al. 2018)
23. Log Koc of Pesticides (Gramatica et al. 2007a)
24. Nitro PAH Mutagenicity (Gramatica et al. 2007b)
25. *Pimephales promelas* tox (Papa et al. 2005b)
26. Persistence Bioaccumulation Toxicity (PBT) Index (Papa and Gramatica 2010)
27. Personal Care Products (PCP) Aquatic Toxicity Index-ATI (Gramatica et al. 2016)
28. PCP *D.magna* acute tox (Gramatica et al. 2016)
29. PCP *P.promelas* acute tox LogP-based (Gramatica et al. 2016)
30. PCP *P.promelas* acute tox (Gramatica et al. 2016)

31. PCP *P.subcapitata* acute tox (Gramatica et al. 2016)
32. PerFluorinated Chemicals (PFC) Mouse Inhalation tox (Bhhatarai and Gramatica 2010)
33. PFC Rat Inhalation tox (Bhhatarai and Gramatica 2010)
34. PFC Rat Oral tox (Bhhatarai and Gramatica 2011b)
35. PFC Sw (Bhhatarai and Gramatica 2011c)
36. PFC VP (Bhhatarai and Gramatica 2011c)
37. Pharm. Aquatic Toxicity Index-ATI (Sangion and Gramatica 2016a)
38. Pharm. *D.magna* acute tox (Sangion and Gramatica 2016a)
39. Pharm. O.mykiss acute tox (Sangion and Gramatica 2016a)
40. Pharm. *P.promelas* acute tox (Sangion and Gramatica 2016a)
41. Pharm. *P.subcapitata* acute tox (Sangion and Gramatica 2016a)
42. PPCP intertox *D.magna-O.mykiss* (Sangion and Gramatica 2016b)
43. PPCP intertox *D.magna-P.promelas* (Sangion and Gramatica 2016b)
44. PPCP intertox *O.mykiss-P.promelas* (Sangion and Gramatica 2016b)
45. PPCP intertox P.promelas-O.mykiss (Sangion and Gramatica 2016b)

## *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 modeling method. However, any personal MLR model, even if developed by other software, can be analyzed by the plots available in QSARINS as well as validated by several statistical validation parameters (both for internal and external validation: see above list).

Other chemometric tools (Principal Component Analysis (PCA), Multicriteria Decision Macking (MCDM)) for explorative analysis and ranking are also implemented, **therefore QSARINS is not limited to QSAR studies.**

It is also important to note that not only chemicals, but any kind of objects can be analyzed or modeled in a multivariate way.

## *Bibliography*


Bhhatarai B, Gramatica P (2011a) Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning. Water Res 45:1463–1471. doi: 10.1016/j.watres.2010.11.006

Bhhatarai B, Gramatica P (2010) Per- and Polyfluoro Toxicity (LC50 Inhalation) Study in Rat and Mouse Using QSAR Modeling. Chem Res Toxicol 23:528–539. doi: 10.1021/tx900252h

Bhhatarai B, Gramatica P (2011b) Oral LD50 toxicity modeling and prediction of per- and polyfluorinated chemicals on rat and mouse. Mol Divers 15:467–476. doi: 10.1007/s11030-010-9268-z

Bhhatarai B, Gramatica P (2011c) Prediction of Aqueous Solubility, Vapor Pressure and Critical Micelle Concentration for Aquatic Partitioning of Perfluorinated Chemicals. Environ Sci Technol 45:8120–8128. doi: 10.1021/es101181g

Cassani S, Kovarich S, Papa E, et al (2013) Daphnia and fish toxicity of (benzo)triazoles: Validated QSAR models, and interspecies quantitative activity–activity modelling. J Hazard Mater 258–259:50–60. doi: 10.1016/j.jhazmat.2013.04.025

Chirico N, Gramatica P (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 51:2320–2335. doi: 10.1021/ci200211n

Chirico N, Gramatica P (2012) Real External Predictivity of QSAR Models. Part 2. New Intercomparable Thresholds for Different Validation Criteria and the Need for Scatter Plot Inspection. J Chem Inf Model 52:2044–2058. doi: 10.1021/ci300084j

Gramatica P (2007) Principles of QSAR models validation: internal and external. Qsar Comb Sci 26:694–701. doi: 10.1002/qsar.200610151

Gramatica P (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. In: Puzyn T, Leszczynski J, Cronin MT (eds) Recent Advances in QSAR Studies. Springer Netherlands, pp 327–366

Gramatica P (2012) Modelling Chemicals in the Environment. In: Livingstone D, Davis A (eds) Drug Design Strategies Quantitative Approaches. RSC Publishing

Gramatica P (2013) On the Development and Validation of QSAR Models. In: Reisfeld B, Mayeno AN (eds) Computational Toxicology. Humana Press, pp 499–526

Gramatica P (2014) External Evaluation of QSAR Models, in Addition to Cross-Validation: Verification of Predictive Capability on Totally New Chemicals. Mol Inform 33:311–314

Gramatica P (2016) Prioritization of Chemicals Based on Chemoinformatic Analysis. In: Leszczynski J (ed) Handbook of Computational Chemistry. Springer Netherlands, pp 1–33

Gramatica P, Cassani S, Roy PP, et al (2012) QSAR modeling is not “push a button and find a correlation”: a case study of toxicity of (benzo-)triazoles on algae. Mol Inf 31:817–835. doi: 10.1002/minf.201200075

Gramatica P, Cassani S, Sangion A (2016) Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternatives’ design. Green Chem 18:4393 – 4406. doi: 10.1039/C5GC02818C

Gramatica P, Giani E, Papa E (2007a) Statistical external validation and consensus modeling: A QSPR case study for K-oc prediction. J Mol Graph Model 25:755–766. doi: 10.1016/j.jmgm.2006.06.005

Gramatica P, Papa E (2007) Screening and ranking of POPs for global half-life: QSAR approaches for prioritization based on molecular structure. Environ Sci Technol 41:2833–2839. doi: 10.1021/es061773b

Gramatica P, Pilutti P, Papa E (2007b) Approaches for externally validated QSAR modelling of Nitrated Polycyclic Aromatic Hydrocarbon mutagenicity. SAR QSAR Environ Res 18:169–178. doi: 10.1080/10629360601054388

Gramatica P, Sangion A (2016) A Historical Excursus on the Statistical Validation Parameters for QSAR Models: A Clarification Concerning Metrics and Terminology. J Chem Inf Model 56:1127–1131. doi: 10.1021/acs.jcim.6b00088

Li J, Gramatica P (2010) The importance of molecular structures, endpoints’ values, and predictivity parameters in QSAR research: QSAR analysis of a series of estrogen receptor binders. Mol Divers 14:687–696. doi: 10.1007/s11030-009-9212-2

Papa E, Battaini F, Gramatica P (2005a) Ranking of aquatic toxicity of esters modelled by QSAR. Chemosphere 58:559–570. doi: 10.1016/j.chemosphere.2004.08.003

Papa E, Gramatica P (2010) QSPR as a support for the EU REACH regulation and rational design of environmentally safer chemicals: PBT identification from molecular structure. Green Chem 12:836–843. doi: 10.1039/B923843C

Papa E, Kovarich S, Gramatica P (2009) Development, Validation and Inspection of the Applicability Domain of QSPR Models for Physicochemical Properties of Polybrominated Diphenyl Ethers. QSAR Comb Sci 28:790–796. doi: 10.1002/qsar.200860183

Papa E, Sangion A, Arnot JA, Gramatica P (2018) Development of human biotransformation QSARs and application for PBT assessment refinement. Food Chem Toxicol 112:535–543. doi: 10.1016/j.fct.2017.04.016

Papa E, van der Wal L, Arnot JA, Gramatica P (2014) Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. Sci Total Env 470–471:1040–1046

Papa E, Villa F, Gramatica P (2005b) Statistically validated QSARs, based on theoretical descriptors, for modeling aquatic toxicity of organic chemicals in Pimephales promelas (fathead minnow). J Chem Inf Model 45:1256–1266. doi: 10.1021/ci050212l

Sangion A, Gramatica P (2016a) Ecotoxicity interspecies QAAR models from Daphnia toxicity of pharmaceuticals and personal care products. SAR QSAR Environ Res 0:1–18. doi: 10.1080/1062936X.2016.1233139

Sangion A, Gramatica P (2016b) Hazard of pharmaceuticals for aquatic environment: Prioritization by structural approaches and prediction of ecotoxicity. Environ Int 95:131–143. doi: 10.1016/j.envint.2016.08.008

Tropsha A, Gramatica P, Gombar VK (2003) The importance of being earnest: Validation is the absolute essential for successful application and interpretation of QSPR models. Qsar Comb Sci 22:69–77. doi: 10.1002/qsar.200390007

**QSARINS is currently used by the Insubria group and several international QSAR groups: about 300 free licenses were active into 2017.**

## QSARINS citations

**QSARINS has been cited in the following peer-reviewed publications (February 2018):**


Aalizadeh R, Pourbasheer E, Ganjali MR (2015) Analysis of B-Raf inhibitors using 2D and 3D-QSAR, molecular docking and pharmacophore studies. Mol Divers 19:915–930. doi: 10.1007/s11030-015-9626-y

Ahmed L, Rasulev B, Kar S, et al (2017) Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale 9:10263–10276. doi: 10.1039/c7nr00770a

Ambure P, Aher RB, Roy K (2014) Recent Advances in the Open Access Cheminformatics Toolkits, Software Tools, Workflow Environments, and Databases. In: Computer-Aided Drug Discovery. Springer, pp 257–296

Amrani LK, Tazir A, Mazouni NS (2015) Crop protection and preservation of environment: evaluation in vivo of bisacylhydrazine ecdysteroid mimics (RH-5849 and RH-5992) on pupae of Ephestia kuehniella. In: 18th International Symposium on Environmental Pollution and its Impact on Life in the Mediterranean Region. p 51

Antypenko LM, Kovalenko SI, Los' TS, Rebec' OL (2017) Synthesis and Characterization of Novel N-(Phenyl, Benzyl, Hetaryl)-2-([1,2,4]Triazolo[1,5-c]Quinazolin-2-ylthio)Acetamides by Spectral Data, Antimicrobial Activity, Molecular Docking and QSAR Studies. J Heterocycl Chem 54:1267–1278. doi: 10.1002/jhet.2702

Antypenko OM, Kovalenko SI, Karpenko OV, et al (2016) Synthesis, Anticancer, and QSAR Studies of 2-Alkyl(aryl,hetaryl)quinazolin-4(3H)-thione's and [1,2,4]Triazolo[1,5-c]quinazoline-2-thione's Thioderivatives. Helv Chim Acta 99:621–631. doi: 10.1002/hlca.201600062

Aswathy L, Jisha RS, Masand VH, et al (2016) Computational strategies to explore antimalarial thiazine alkaloid lead compounds based on an Australian marine sponge Plakortis Lita. Journal of Biomolecular Structure and Dynamics 1–23. doi: 10.1080/07391102.2016.1220870

Aytac PS, Durmaz I, Houston DR, et al (2016) Novel triazolothiadiazines act as potent anticancer agents in liver cancer cells through Akt and ASK-1 proteins. Bioorg Med Chem 24:858–872. doi: 10.1016/j.bmc.2016.01.013

Bahmani A, Saaidpour S, Rostami A (2017) A Simple, Robust and Efficient Computational Method for n-Octanol/Water Partition Coefficients of Substituted Aromatic Drugs. Scientific Reports 7:5760. doi: 10.1038/s41598-017-05964-z

Barycki M, Sosnowska A, Gajewicz A, et al (2016a) Temperature-dependent structure-property modeling of viscosity for ionic liquids. Fluid Phase Equilib 427:9–17. doi:

10.1016/j.fluid.2016.06.043

Barycki M, Sosnowska A, Piotrowska M, et al (2016b) ILPC: simple chemometric tool supporting the design of ionic liquids. J Cheminformatics 8:40. doi: 10.1186/s13321-016-0152-4

Barycki M, Sosnowska A, Puzyn T (2017) Which structural features stand behind micelization of ionic liquids? Quantitative Structure-Property Relationship studies. J Colloid Interface Sci 487:475–483. doi: 10.1016/j.jcis.2016.10.066

Beier R, Labudde D (2016) Numeric promoter description - A comparative view on concepts and general application. J Mol Graph 63:65–77. doi: 10.1016/j.jmgm.2015.11.011

Beiknejad D, Chaichi MJ, Fatemi MH (2016) Prediction of photolysis half-lives of dihydroindolizines by genetic algorithm-multiple linear regression (GA-MLR). J Phys Org Chem 29:312–320. doi: 10.1002/poc.3540

Biswas S, Kayaleh R, Pillai GG, et al (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 20:8189–8198. doi: 10.1002/chem.201400125

Bukhari SNA, Jantan I, Masand VH, et al (2014) Synthesis of alpha, beta-unsaturated carbonyl based compounds as acetylcholinesterase and butyrylcholinesterase inhibitors: Characterization, molecular modeling, QSAR studies and effect against amyloid beta-induced cytotoxicity. Eur J Med Chem 83:355–365. doi: 10.1016/j.ejmech.2014.06.034

Cañizares-Carmenate Y, Hernandez-Morfa M, Torrens F, et al (2017) Larvicidal activity prediction against Aedes aegypti mosquito using computational tools. Journal of vector borne diseases 54:164

Cañizares-Carmenate Y, Mena-Ulecia K, Perera-Sardiña Y, et al (2016) An approach to identify new antihypertensive agents using Thermolysin as model: in silico study based on QSARINS and Docking. Arabian Journal of Chemistry. doi: doi.org/10.1016/j.arabjc.2016.10.003

Caruso E, Gariboldi M, Sangion A, et al (2017) Synthesis, photodynamic activity, and quantitative structure-activity relationship modelling of a series of BODIPYs. Journal of Photochemistry and Photobiology B: Biology 167:269–281. doi: 10.1016/j.jphotobiol.2017.01.012

Cassani S, Gramatica P (2015) Identification of potential PBT behavior of personal care products by structural approaches. Sustainable Chemistry and Pharmacy 1:19–27. doi: 10.1016/j.scp.2015.10.002

Cassano A, Marchese Robinson RL, Palczewska A, et al (2016) Comparing the CORAL and random forest approaches for modelling the in vitro cytotoxicity of silica nanomaterials. Altern Lab Anim 44:533–556

Ceriani L, Papa E, Kovarich S, et al (2015) Modeling ready biodegradability of fragrance materials. Environ Toxicol Chem 34:1224–1231. doi: 10.1002/etc.2926

Chayawan, Vikas (2015) Externally predictive single-descriptor based QSPRs for physico-chemical properties of polychlorinated-naphthalenes: Exploring relationships of log S-W, log K-OA, and log K-OW with electron-correlation. J Hazard Mater 296:68–81. doi:

10.1016/j.jhazmat.2015.04.028

Chayawan, Vikas (2016) Quantum-mechanical parameters for the risk assessment of multi-walled carbon-nanotubes: A study using adsorption of probe compounds and its application to biomolecules. Environ Pollut 218:615–624. doi: 10.1016/j.envpol.2016.07.045

Crisan L, Funar-Timofei S, Borota A (2017) Qsar and ligand-based pharmacophore models of dibenzoylhydrazines with insecticide activity against the silkworm Bombyx mori l. Rev Roum Chim 62:699–706

Crisan L, Iliescu S, Funar-Timofei S (2016) Structure-flammability relationship study of phosphoester dimers by MLR and PLS. Polimeros 26:129–136. doi: 10.1590/0104-1428.2306

de Campos LJ, de Melo EB (2014) Modeling structure–activity relationships of prodiginines with antimalarial activity using GA/MLR and OPS/PLS. Journal of Molecular Graphics and Modelling 54:19–31. doi: doi.org/10.1016/j.jmgm.2014.08.004

Dems MAE, Laib S, Latelli N, Ouddai N (2017) A DFT-based Quantitative structure activity relationship Study of organometallic estradiol derivatives. 10:483–487

Devi J, Devi S, Kumar A (2016a) Synthesis, antibacterial evaluation and QSAR analysis of Schiff base complexes derived from [2,2 ’-(ethylenedioxy)bis(ethylamine)] and aromatic aldehydes. MedChemComm 7:932–947. doi: 10.1039/c5md00554j

Devi J, Devi S, Kumar A (2016b) Synthesis, characterization, and quantitative structure-activity relationship studies of bioactive dehydroacetic acid and amino ether Schiff base complexes. Heteroatom Chem 27:361–371. doi: 10.1002/hc.21347

Ding Y-L, Lyu Y-C, Leong MK (2016) In silico prediction of the mutagenicity of nitroaromatic compounds using a novel two-QSAR approach. Toxicology in Vitro 40:102–114. doi: doi.org/10.1016/j.tiv.2016.12.013

Dong J, Yao Z-J, Zhu M-F, et al (2017) ChemSAR: an online pipelining platform for molecular SAR modeling. Journal of cheminformatics 9:27. doi: doi.org/10.1186/s13321-017-0215-1

Doucet JP, Papa E, Doucet-Panaye A, Devillers J (2017) QSAR models for predicting the toxicity of piperidine derivatives against Aedes aegypti. SAR QSAR Environ Res 28:451–470. doi: 10.1080/1062936X.2017.1328855

Drgan V, Zuperl S, Vracko M, et al (2016) Robust modelling of acute toxicity towards fathead minnow (Pimephales promelas) using counter-propagation artificial neural networks and genetic algorithm. SAR QSAR Environ Res 27:501–519. doi: 10.1080/1062936X.2016.1196388

Erzincan P, Sacan MT, Yuce-Dursun B, et al (2015) QSAR models for antioxidant activity of new coumarin derivatives. SAR QSAR Environ Res 26:721–737. doi: 10.1080/1062936X.2015.1088571

Fu Y, Sun Y-N, Cao H-F, et al (2017) New Research for Quinazoline-2,4-diones as HPPD Inhibitors Based on 2D-MLR and 3D-QSAR Models. Comb Chem High Throughput Screen 20:748–759. doi: 10.2174/1386207320666170622073738

Funar-Timofei S, Avram S, Borota A (2016) Structure-toxicity study of some pyrethroidal ester insecticides. doi: doi:10.3390/ecsoc-17-e012

Funar-Timofei S, Borota A, Crisan L (2017) Combined molecular docking and QSAR study of fused heterocyclic herbicide inhibitors of D1 protein in photosystem II of plants. Molecular diversity 21:437–454. doi: doi.org/10.1007/s11030-017-9735-x

Funar-Timofei S, Iliescu S, Suzuki T (2014) Correlations of limiting oxygen index with structural polyphosphoester features by QSPR approaches. Struct Chem 25:1847–1863. doi: 10.1007/s11224-014-0474-7

Furuhama A, Hayashi TI, Tatarazako N (2016) Acute to chronic estimation of Daphnia magna toxicity within the QSAAR framework. SAR QSAR Environ Res 27:833–850. doi: 10.1080/1062936X.2016.1243151

Gajewicz A (2018) How to judge whether QSAR/read-across predictions can be trusted: a novel approach for establishing a model's applicability domain. Environmental Science: Nano. doi: 10.1039/C7EN00774D

Garg R, Smith CJ (2014) Predicting the bioconcentration factor of highly hydrophobic organic chemicals. Food Chem Toxicol 69:252–259. doi: 10.1016/j.fct.2014.03.035

Gooch A, Sizochenko N, Rasulev B, et al (2017a) In Vivo Toxicity of Nitroaromatics: A Comprehensive Quantitative Structure-Activity Relationship Study. Environ Toxicol Chem 36:2227–2233. doi: 10.1002/etc.3761

Gooch A, Sizochenko N, Sviatenko L, et al (2017b) A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds. SAR and QSAR in Environmental Research 28:133–150. doi: dx.doi.org/10.1080/1062936X.2017.1286687

Gramatica P (2014) External Evaluation of QSAR Models, in Addition to CrossValidation: Verification of Predictive Capability on Totally New Chemicals. Mol Inf 33:311–314. doi: 10.1002/minf.201400030

Gramatica P (2016) Prioritization of Chemicals Based on Chemoinformatic Analysis. Handbook of Computational Chemistry 1–33

Gramatica P, Cassani S, Chirico N (2014) QSARINS-Chem: Insubria Datasets and New QSAR/QSPR Models for Environmental Pollutants in QSARINS. J Comput Chem 35:1036–1044. doi: 10.1002/jcc.23576

Gramatica P, Cassani S, Sangion A (2015a) PBT assessment and prioritization by PBT Index and consensus modeling: Comparison of screening results from structural models. Environ Int 77:25–34. doi: 10.1016/j.envint.2014.12.012

Gramatica P, Cassani S, Sangion A (2016a) Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternatives' design. Green Chem 18:4393 – 4406. doi: 10.1039/C5GC02818C

Gramatica P, Cassani S, Sangion A (2016b) Are some "safer alternatives" hazardous as PBTs? The

case study of new flame retardants. Journal of Hazardous Materials 306:237–246. doi: 10.1016/j.jhazmat.2015.12.017

Gramatica P, Cassani S, Sangion A, Papa E (2015b) Screening and prioritization of chemicals for REACH: The cumulative PBT Index model in QSARINS. Toxicol Lett 238:S338–S338. doi: 10.1016/j.toxlet.2015.08.964

Gramatica P, Papa E, Sangion A (2018) QSAR modeling of cumulative environmental end-points for the prioritization of hazardous chemicals. Environmental Science: Processes & Impacts 20:38–47. doi: 10.1039/c7em00519a

Gramatica P, Sangion A (2016) A Historical Excursus on the Statistical Validation Parameters for QSAR Models: A Clarification Concerning Metrics and Terminology. J Chem Inf Model 56:1127–1131. doi: 10.1021/acs.jcim.6b00088

Grzonkowska M, Sosnowska A, Barycki M, et al (2016) How the structure of ionic liquid affects its toxicity to Vibrio fischeri? Chemosphere 159:199–207. doi: 10.1016/j.chemosphere.2016.06.004

Hamadanian M, Keshavarz MH, Nazari B, Mohebbi M (2016) Reliable method for safety assessment of melting points of energetic compounds. Process Saf Environ Protect 103:10–22. doi: 10.1016/j.psep.2016.06.025

Huang L, Fantke P, Ernstoff A, Jolliet O (2017) A quantitative property-property relationship for the internal diffusion coefficients of organic compounds in solid materials. Indoor air 27:1128–1140. doi: DOI: 10.1111/ina.12395

Jabeen F, Chen M, Rasulev B, et al (2017) Refractive indices of diverse data set of polymers: A computational QSPR based study. Computational Materials Science 137:215–224. doi: doi.org/10.1016/j.commatsci.2017.05.022

Jagiello K, Grzonkowska M, Swirog M, et al (2016) Advantages and limitations of classic and 3D QSAR approaches in nano-QSAR studies based on biological activity of fullerene derivatives. J Nanopart Res 18:256. doi: 10.1007/s11051-016-3564-1

Jimena Martinez M, Ponzoni I, Diaz MF, et al (2015) Visual analytics in cheminformatics: user-supervised descriptor selection for QSAR methods. J Cheminformatics 7:39. doi: 10.1186/s13321-015-0092-4

Judycka-Proma U, Bober L, Gajewicz A, et al (2015) Chemometric analysis of correlations between electronic absorption characteristics and structural and/or physicochemical parameters for ampholytic substances of biological and pharmaceutical relevance. Spectroc Acta Pt A-Molec Biomolec Spectr 138:700–710. doi: 10.1016/j.saa.2014.11.067

Jukić M, Rastija V, Opačak-Bernardi T, et al (2017) Antitumor activity of 3, 4-ethylenedioxythiophene derivatives and quantitative structure-activity relationship analysis. Journal of Molecular Structure 1133:66–73. doi: dx.doi.org/10.1016/j.molstruc.2016.11.074

Karabulut S, Sizochenko N, Orhan A, Leszczynski J (2016) A DFT-based QSAR study on inhibition of human dihydrofolate reductase. J Mol Graph 70:23–29. doi: 10.1016/j.jmgm.2016.09.005

Kolaric A, Minovski N (2017) Structure-based design of novel combinatorially generated NBTIs as potential DNA gyrase inhibitors against various Staphylococcus aureus mutant strains. Molecular BioSystems 13:1406–1420. doi: 10.1039/C7MB00168A

Lata S, Vikas (2017) Dispersibility of carbon nanotubes in organic solvents: do we really have predictive models? Journal of Nanoparticle Research 19:211. doi: 10.1007/s11051-017-3883-x

Li J, Bai F, Liu H, Gramatica P (2015a) Ligand Efficiency Outperforms pIC(50) on Both 2D MLR and 3D CoMFA Models: A Case Study on AR Antagonists. Chem Biol Drug Des 86:1501–1517. doi: 10.1111/cbdd.12619

Li J, Li S, Bai C, et al (2013) Structural requirements of 3-carboxyl-4 (1H)-quinolones as potential antimalarials from 2D and 3D QSAR analysis. Journal of Molecular Graphics and Modelling 44:266–277. doi: doi.org/10.1016/j.jmgm.2013.07.004

Li S, Li J, Ning L, et al (2015b) In Silico Identification of Protein S-Palmitoylation Sites and Their Involvement in Human Inherited Disease. J Chem Inf Model 55:2015–2025. doi: 10.1021/acs.jcim.5b00276

Liu L, Brailsford JA (2015) Protein Ligation and Total Synthesis: I. Springer

Maria Olguin CJ, Sampaio SC, dos Reis RR (2017) Statistical equivalence of prediction models of the soil sorption coefficient obtained using different log P algorithms. Chemosphere 184:498–504. doi: 10.1016/j.chemosphere.2017.06.027

Martincic R, Kuzmanovski I, Wagner A, Novic M (2015) Development of models for prediction of the antioxidant activity of derivatives of natural compounds. Anal Chim Acta 868:23–35. doi: 10.1016/j.aca.2015.01.050

Martincic R, Venko K, Zuperl S, Novic M (2014) Chemometrics approach for the prediction of structure-activity relationship for membrane transporter bilitranslocase. SAR QSAR Environ Res 25:853–872. doi: 10.1080/1062936X.2014.962082

Masand VH, El-Sayed NNE, Mahajan DT, Rastija V (2017a) QSAR analysis for 6-arylpyrazine-2-carboxamides as Trypanosoma brucei inhibitors. SAR QSAR Environ Res 28:165–177. doi: 10.1080/1062936X.2017.1292407

Masand VH, El-Sayed NNE, Mahajan FT, et al (2017b) QSAR modeling for anti-human African trypanosomiasis activity of substituted 2-Phenylimidazopyridines. J Mol Struct 1130:711–718. doi: 10.1016/j.molstruc.2016.11.012

Masand VH, Mahajan DT, Gramatica P, Barlow J (2014) Tautomerism and multiple modelling enhance the efficacy of QSAR: antimalarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl. Med Chem Res 23:4825–4835. doi: 10.1007/s00044-014-1043-8

Masand VH, Mahajan DT, Maldhure AK, Rastija V (2016) Quantitative structure–activity relationships (QSARs) and pharmacophore modeling for human African trypanosomiasis (HAT) activity of pyridyl benzamides and 3-(oxazolo [4, 5-b] pyridin-2-yl) anilides. Medicinal

chemistry research 25:2324–2334. doi: 10.1007/s00044-016-1664-1

Masand VH, Mahajan DT, Nazeruddin GM, et al (2015a) Effect of information leakage and method of splitting (rational and random) on external predictive ability and behavior of different statistical parameters of QSAR model. Med Chem Res 24:1241–1264. doi: 10.1007/s00044-014-1193-8

Masand VH, Mahajan DT, Nazeruddin GM, et al (2015b) 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. Medicinal Chemistry Research 24:1241–1264. doi: 10.1007/s00044-014-1193-8

Masand VH, Rastija V (2017) PyDescriptor: A new PyMOL plugin for calculating thousands of easily understandable molecular descriptors. Chemometrics Intell Lab Syst 169:12–18. doi: 10.1016/j.chemolab.2017.08.003

Mikolajczyk A, Gajewicz A, Rasulev B, et al (2015) Zeta Potential for Metal Oxide Nanoparticles: A Predictive Model Developed by a Nano-Quantitative Structure-Property Relationship Approach. Chem Mat 27:2400–2407. doi: 10.1021/cm504406a

Mikolajczyk A, Malankowska A, Nowaczyk G, et al (2016) Combined experimental and computational approach to developing efficient photocatalysts based on Au/Pd-TiO2 nanoparticles. Environ-Sci Nano 3:1425–1435. doi: 10.1039/c6en00232c

Molnar M, Komar M, Brahmbhatt H, et al (2017) Deep Eutectic Solvents as Convenient Media for Synthesis of Novel Coumarinyl Schiff Bases and Their QSAR Studies. Molecules 22:1482. doi: 10.3390/molecules22091482

Nazari B, Hamadanian M, Keshavarz MH, Rezaei J (2016) New method for assessment of melting points of organic azides using their molecular structures. Fluid Phase Equilib 427:27–34. doi: 10.1016/j.fluid.2016.06.051

Nosulenko IS, Voskoboynik OY, Antypenko OM, et al (2015) Methodology for prediction of anticancer action of (2-oxo-2H-[1, 2, 4] triazino [2, 3-c]-quinazolin-6-yl) thiones via QSAR and docking studies

Önlü S, Saçan MT (2016a) An in silico algal toxicity model with a wide applicability potential for industrial chemicals and pharmaceuticals. Environmental Toxicology and Chemistry. doi: 10.1002/etc.3620

Önlü S, Saçan MT (2016b) An in silico approach to cytotoxicity of pharmaceuticals and personal care products on the rainbow trout liver cell line RTL-W1. Environmental Toxicology and Chemistry. doi: 10.1002/etc.3663

Önlü S, Türker Saçan M (2017) Impact of geometry optimization methods on QSAR modelling: A case study for predicting human serum albumin binding affinity. SAR and QSAR in Environmental Research 28:491–509. doi: 10.1080/1062936X.2017.1343253

Orucu E, Tugcu G, Sacan MT (2014) Molecular structure-adsorption study on current textile dyes. SAR QSAR Environ Res 25:983–998. doi: 10.1080/1062936X.2014.976266

Panda SS, Jones RA, Hall CD, Katritzky AR (2014) Applications of Chemical Ligation in Peptide Synthesis via Acyl Transfer. In: Protein Ligation and Total Synthesis I. Springer, pp 229–265

Papa E, Arnot JA, Sangion A, Gramatica P (2017a) In Silico Approaches for the Prediction of In Vivo Biotransformation Rates. In: Advances in QSAR Modeling. Springer, pp 425–451

Papa E, Doucet JP, Doucet-Panaye A (2015) Linear and non-linear modelling of the cytotoxicity of TiO2 and ZnO nanoparticles by empirical descriptors. SAR QSAR Environ Res 26:647–665. doi: 10.1080/1062936X.2015.1080186

Papa E, Doucet JP, Doucet-Panaye A (2016a) Computational approaches for the prediction of the selective uptake of magnetofluorescent nanoparticles into human cells. RSC Adv 6:68806–68818. doi: 10.1039/c6ra07898b

Papa E, Doucet JP, Sangion A, Doucet-Panaye A (2016b) Investigation of the influence of protein corona composition on gold nanoparticle bioactivity using machine learning approaches. SAR QSAR Environ Res 27:521–538. doi: 10.1080/1062936X.2016.1197310

Papa E, Sangion A, Arnot JA, Gramatica P (2017b) Development of human biotransformation QSARs and application for PBT assessment refinement. Food and Chemical Toxicology. doi: 10.1016/j.fct.2017.04.016

Papa E, van der Wal L, Arnot JA, Gramatica P (2014) Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. Sci Total Environ 470:1040–1046. doi: 10.1016/j.scitotenv.2013.10.068

Papadaki KC, Karakitsios SP, Sarigiannis DA (2017) Modeling of adipose/blood partition coefficient for environmental chemicals. Food Chem Toxicol 110:274–285. doi: 10.1016/j.fct.2017.10.044

Paterno A, Goracci L, Scire S, Musumarra G (2017) Modeling from Theory and Modeling from Data: Complementary or Alternative Approaches? The Case of Ionic Liquids. ChemistryOpen 6:90–101. doi: 10.1002/open.201600119

Pillai GG (2015) Computational Modelling of Diverse Chemical, Biochemical and Biomedical Properties. PhD Thesis

Pillai GG, Mederos L, Panda CS, et al (2016) Robust Modeling and Scaffold Hopping: Case Study Based on HIV Reverse Transcriptase Inhibitors Type-1 Data. Med Chem 12:513–526. doi: 10.2174/1573406411666151005110141

Pourbasheer E, Aalizadeh R, Ardabili JS, Ganjali MR (2015) QSPR study on solubility of some fullerenes derivatives using the genetic algorithms - Multiple linear regression. J Mol Liq 204:162–169. doi: 10.1016/j.molliq.2015.01.028

Putz MV, Dudas NA, Isvoran A (2015) Double Variational Binding-(SMILES) Conformational Analysis by Docking Mechanisms for Anti-HIV Pyrimidine Ligands. Int J Mol Sci 16:19553–19601. doi: 10.3390/ijms160819553

Qin L, Zhang X, Chen Y, et al (2017) Predictive QSAR Models for the Toxicity of Disinfection Byproducts. Molecules 22:1671. doi: 10.3390/molecules22101671

Racz A, Bajusz D, Heberger K (2015) Consistency of QSAR models: Correct split of training and test sets, ranking of models and performance parameters. SAR QSAR Environ Res 26:683–700. doi: 10.1080/1062936X.2015.1084647

Rastija V, Agic D, Tomic S, et al (2015) Synthesis, QSAR, and Molecular Dynamics Simulation of Amidino-substituted Benzimidazoles as Dipeptidyl Peptidase III Inhibitors. Acta Chim Slov 62:867–878

Rastija V, Masand VH (2014) QSAR of Antitrypanosomal Activities of Polyphenols and their Analogues Using Multiple Linear Regression and Artificial Neural Networks. Comb Chem High Throughput Screen 17:709–717. doi: 10.2174/1386207317666140804161605

Rasulev B, Jabeen F, Stafslien S, et al (2017) Polymer Coating Materials and Their Fouling Release Activity: A Cheminformatics Approach to Predict Properties. ACS Appl Mater Interfaces 9:1781–1792. doi: 10.1021/acsami.6b12766

Rath EC, Bai Y (2016) Quantitative Structure-Activity Relation Study of Quaternary Ammonium Compounds in Pathogen Control: Computational Methods for the Discovery of Food Antimicrobials. Chemical Informatics. doi: 10.21767/2470-6973.100017

Rath EC, Gill H, Bai Y (2017) Identification of potential antimicrobials against Salmonella typhimurium and Listeria monocytogenes using Quantitative Structure-Activity Relation modeling. PloS one 12:1–17. doi: doi.org/10.1371/journal.pone.0189580

Ravichandran V, Shalini S, Venkateskumar K, Dhanaraj SA (2016a) Exploring the Structural Insights of Indole-7-Carboxamides as Anti-Hiv Agents. Farmacia 64:745–756. doi: doi.org/10.1016/j.chemolab.2016.03.017

Ravichandran V, Venkateskumar K, Shalini S, Harish R (2016b) Exploring the structure-activity relationship of oxazolidinones as HIV-1 protease inhibitors-QSAR and pharmacophore modelling studies. Chemometrics Intell Lab Syst 154:52–61. doi: 10.1016/j.chemolab.2016.03.017

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

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

Reenu, Vikas (2015b) Exploring the role of quantum chemical descriptors in modeling acute toxicity of diverse chemicals to Daphnia magna. J Mol Graph 61:89–101. doi: 10.1016/j.jmgm.2015.06.009

Reenu, Vikas (2016) Evaluating the role of electron-correlation in the external prediction of the toxicity of nitrobenzenes towards Tetrahymena pyriformis. New J Chem 40:2343–2353. doi: 10.1039/c5nj02552d

Rehman TU, Khan IU, Ashraf M, et al (2017) An Efficient Synthesis of bi-Aryl Pyrimidine Heterocycles:

Potential New Drug Candidates to Treat Alzheimer's Disease. Archiv der Pharmazie 350:. doi: 10.1002/ardp.201600304

Ruusmann V, Sild S, Maran U (2015) QSAR DataBank repository: open and linked qualitative and quantitative structure-activity relationship models. J Cheminformatics 7:32. doi: 10.1186/s13321-015-0082-6

Rybinska A, Sosnowska A, Barycki M, Puzyn T (2016a) Geometry optimization method versus predictive ability in QSPR modeling for ionic liquids. J Comput-Aided Mol Des 30:165–176. doi: 10.1007/s10822-016-9894-3

Rybinska A, Sosnowska A, Grzonkowska M, et al (2016b) Filling environmental data gaps with QSPR for ionic liquids: Modeling n-octanol/water coefficient. J Hazard Mater 303:137–144. doi: 10.1016/j.jhazmat.2015.10.023

Saaidpour S (2016) Quantitative Modeling for Prediction of Critical Temperature of Refrigerant Compounds. Phys Chem Res 4:61–71. doi: 10.22036/pcr.2016.11759

Şahin AD, Saçan MT (2018) Understanding the toxic potencies of xenobiotics inducing TCDD/TCDF-like effects. SAR QSAR Environ Res 1–15. doi: doi.org/10.1080/1062936X.2017.1414075

Sangion A, Gramatica P (2016a) Ecotoxicity interspecies QAAR models from Daphnia toxicity of pharmaceuticals and personal care products. SAR QSAR Environ Res 27:781–798. doi: 10.1080/1062936X.2016.1233139

Sangion A, Gramatica P (2016b) Hazard of pharmaceuticals for aquatic environment: Prioritization by structural approaches and prediction of ecotoxicity. Environ Int 95:131–143. doi: 10.1016/j.envint.2016.08.008

Sangion A, Gramatica P (2016c) PBT assessment and prioritization of contaminants of emerging concern: Pharmaceuticals. Environ Res 147:297–306. doi: 10.1016/j.envres.2016.02.021

Shaik B, Deeb O, Agrawal VK, Gupta SP (2017) QSAR and Molecular Docking Studies on a Series of Cinnamic Acid Analogues as Epidermal Growth Factor Receptor (EGFR) Inhibitors. Lett Drug Des Discov 14:83–95. doi: 10.2174/1570180813999160721160833

Shaik B, Kaushal T, Agrawal VK (2016) Quantitative structure activity relationship studies on a series of 4-pyridones as antimalerial agents. J Indian Chem Soc 93:871–876

Shao Y, Liu J, Wang M, et al (2014) Integrated QSPR models to predict the soil sorption coefficient for a large diverse set of compounds by using different modeling methods. Atmos Environ 88:212–218. doi: 10.1016/j.atmosenv.2013.12.018

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

Sikorska C, Gajewicz A, Urbaszek P, et al (2016) Efficient way of designing fullerene derivatives based on simplified DFT calculations and QSPR modeling. Chemometrics Intell Lab Syst 152:125–133. doi: 10.1016/j.chemolab.2016.02.003

Sosnowska A, Barycki M, Gajewicz A, et al (2016) Towards the Application of Structure-Property Relationship Modeling in Materials Science: Predicting the Seebeck Coefficient for Ionic Liquid/Redox Couple Systems. ChemPhysChem 17:1591–1600. doi: 10.1002/cphc.201600080

Sosnowska A, Grzonkowska M, Puzyn T (2017) Global versus local QSAR models for predicting ionic liquids toxicity against IPC-81 leukemia rat cell line: The predictive ability. J Mol Liq 231:333–340. doi: 10.1016/j.molliq.2017.02.025

Su E (2015) Parallellization of evoQSAR modeling framework and graphical user interface design using PyQt for drug design. PhD Thesis, San Diego State University

Tarazi H, Abu Odeh R, Al-Qawasmeh R, et al (2017) Design, synthesis and SAR analysis of potent BACE1 inhibitors: Possible lead drug candidates for Alzheimer's disease. Eur J Med Chem 125:1213–1224. doi: 10.1016/j.ejmech.2016.11.021

Tetko IV, Maran U, Tropsha A (2017) Public (Q) SAR Services, Integrated Modeling Environments, and Model Repositories on the Web: State of the Art and Perspectives for Future Development. Mol Inf 36:UNSP 1600082. doi: 10.1002/minf.201600082

Tromelin A (2016) Prediction of perception using structure–activity models. In: Flavor: From Food to Behaviors, Wellbeing and Health. p 181

Tugcu G, Erturk MD, Sacan MT (2017) On the aquatic toxicity of substituted phenols to Chlorella vulgaris: QSTR with an extended novel data set and interspecies models. J Hazard Mater 339:122–130. doi: 10.1016/j.jhazmat.2017.06.027

Tugcu G, Sacan MT (2018) A multipronged QSAR approach to predict algal low-toxic-effect concentrations of substituted phenols and anilines. J Hazard Mater 344:893–901. doi: 10.1016/j.jhazmat.2017.11.033

Veerasamy R, Sivadasan S, Krishnamoorthi V, et al (2016) QSAR study on quinolinecarbaldehyde derivatives as potential anti-tubercular agents. Thai Journal of Pharmaceutical Sciences (TJPS) 40:

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

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 118:239–245. doi: 10.1016/j.chemosphere.2014.08.072

Wang T, Yuan X, Wu M-B, et al (2017a) The advancement of multidimensional QSAR for novel drug discovery-where are we headed? Expert opinion on drug discovery 12:769–784. doi: 10.1080/17460441.2017.1336157

Wang Y, Bai F, Cao H, et al (2015) A Combined Quantitative Structure-Activity Relationship Research

of Quinolinone Derivatives as Androgen Receptor Antagonists. Comb Chem High Throughput Screen 18:834–845. doi: 10.2174/1386207318666150831125750

Wang Y, Han R, Zhang H, et al (2017b) Combined Ligand/Structure-based Virtual Screening and Molecular Dynamics Simulations of Steroidal Androgen Receptor Antagonists. doi: doi.org/10.1155/2017/3572394

Wilde ML, Menz J, Leder C, Kümmerer K (2017) Combination of experimental and in silico methods for the assessment of the phototransformation products of the antipsychotic drug/metabolite Mesoridazine. Science of The Total Environment. doi: doi: 10.1016/j.scitotenv.2017.08.040.

Wyrzykowska E, Mikolajczyk A, Sikorska C, Puzyn T (2016) Development of a novel in silico model of zeta potential for metal oxide nanoparticles: a nano-QSPR approach. Nanotechnology 27:445702. doi: 10.1088/0957-4484/27/44/445702

Xi L, Li S, Yao X, et al (2014) In Silico Study Combining Docking and QSAR Methods on a Series of Matrix Metalloproteinase 13 Inhibitors. Arch Pharm 347:825–833. doi: 10.1002/ardp.201400200

Yousefinejad S, Hemmateenejad B (2015) Chemometrics tools in QSAR/QSPR studies: A historical perspective. Chemometrics and Intelligent Laboratory Systems 149, Part B:177–204. doi: 10.1016/j.chemolab.2015.06.016