

Matteo Cassotti

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Summary

Through my MSc and PhD in chemistry, I gained theoretical knowledge and hands-on experience with computer-based methods to predict the properties of chemical substances (Quantitative Structure-Activity Relationships, QSARs). I had the possibility to expand my knowledge in chemoinformatics and modelling during research periods in Germany and Denmark. My MSc thesis was part of an EU project aimed at designing a new chemical substance for the vulcanization of rubber compounds. Currently, I am a part-time consultant at Bracco Imaging with prime focus on statistical analysis of safety studies. In the spare time, I am taking a specialization in Data Science and programming with Python.

Areas of expertise	Languages
<ul style="list-style-type: none">• Computational chemistry (QSAR/QSPR).• Chemometrics and data analysis.• Molecular descriptors.• Multiple-criteria decision-making.• Virtual screening.	<ul style="list-style-type: none">• Italian: native language.• English: excellent speaking and writing ability.• Danish: elementary understanding.
IT skills	Technical skills
<ul style="list-style-type: none">• Statistical software: MATLAB (proficient), SPSS (good), R and GraphPad (basic).• Chemoinformatics software: Dragon for molecular descriptors (excellent); Leadscope for drug-discovery (good); EPI suite, T.E.S.T., QSAR Toolbox, ToxTree and Vega for property prediction (good); HyperChem and Marvin for designing and optimizing molecules (good), OCHEM database and modelling (good).• Other: KNIME for designing workflows (good), Origin Pro for plotting (good).	<ul style="list-style-type: none">• Modelling chemical properties/activities (regression, classification, clustering).• Programming (MATLAB and R).• Algorithms (e.g. OLS, PLS, kNN, PCA, NN, SVM).• Designing workflows to process data.• Variable selection.• Scientific writing.

Work experience

- 2015
Jan. - now **Consultant** at Bracco Imaging s.p.a. (Italy)
- Statistical analysis of preclinical safety studies.
 - Toxicological screening by computational methods.
- 2012
Apr. - Jul. **Researcher in a Marie-Curie project** at Helmholtz Zentrum München (Germany)
- Designed workflows to process and combine data from different databases.
 - Developed predictive QSAR models with different methods and descriptors.
 - Related model performance to chemical classes.
 - Final report available at: <http://www.eco-itn.eu>.

Academic education and experience

- Jan. 2012 - **Ph.D. in Chemical Sciences** at University of Milano-Bicocca (Italy)

- Mar. 2015
- Prepared datasets using KNIME workflows.
 - Calibrated QSAR regression models for acute aquatic toxicity of chemicals.
 - Improved predictivity of QSAR models by defining the applicability domain.
 - Revised a variable selection method and programmed it in MATLAB. Available at: <http://michem.disat.unimib.it>.
 - Developed classification models for estrogen receptor binding in order to screen 32000 chemicals for the US EPA.
 - Performed SAR and QSAR analysis of tribological properties of lubricants for an oil company.
 - Assistant teacher in chemometrics courses.
 - PhD thesis available at: <http://michem.disat.unimib.it>.
- 2014
Aug.
- Visiting Ph.D. student** at University of Copenhagen (Denmark)
- Comparison of nonlinear regression methods (support vector regression, Gaussian process regression and *k* nearest neighbours) applied to QSAR data.
- 2013
Aug. - Dec.
- Visiting Ph.D. student** at the Technical University of Denmark (Denmark)
- Retrieved and prepared data for acute toxicity of chemicals towards fish.
 - Developed QSAR models using Leadscope software.
- Sep. 2008 -
Oct. 2011
- MSc in Chemical Sciences and Technologies** at University of Milano-Bicocca (Italy)
- Thesis within the European [SafeRubber project](#) aimed at developing a new molecule for rubber vulcanization:
 - Retrieved and analysed data for mechanical and rheological properties of existing accelerator molecules.
 - Calibrated QSAR regression models for rubber properties.
 - Applied QSAR models to screen candidate accelerator molecules.
 - Prioritized candidate molecules for testing.
 - Courses in computational chemistry, bioinformatics and chemometrics.
 - Final grade: 110/110 with honours.
- Sep. 2004 -
Apr. 2008
- BSc in Chemical Sciences and Technologies** at University of Milano-Bicocca (Italy)
- Thesis about the applicability of new molecular descriptors for modelling the binding affinity of flavonoids to the GABA_a and estrogen receptors.
 - Courses in multivariate data analysis and chemometrics.
 - Final grade: 110/110 with honours.

Publications in peer reviewed journals

- 2015
- M. Cassotti, D. Ballabio, R. Todeschini, V. Consonni. A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (*Pimephales promelas*). *SAR QSAR Environ. Res.*, 26 (3), 217-243.
- 2014
- M. Cassotti, V. Consonni, A. Mauri, D. Ballabio. Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards *Daphnia magna*. *SAR QSAR Environ. Res.*, 25 (12), 1013-1036.
 - M. Cassotti, D. Ballabio, V. Consonni, A. Mauri, I.V. Tetko, R. Todeschini. Prediction of acute aquatic toxicity towards *Daphnia magna* by using the GA-*k*NN method. *ATLA-Altern. Lab. Anim.*, 42, 31-41.
 - M. Cassotti, F. Grisoni, R. Todeschini. Reshaped Sequential Replacement algorithm: an efficient approach to variable selection. *Chemometr. Intell. Lab.*, 133, 136-148.
 - F. Grisoni, M. Cassotti, R. Todeschini. Reshaped Sequential Replacement for variable selection in QSPR: comparison with other reference methods. *J. Chemometrics*, 28, 249-259.
 - R. Todeschini, V. Consonni, D. Ballabio, A. Mauri, M. Cassotti, S. Lee, A. West, D. Cartledge. QSPR study of rheological and mechanical properties of Chloroprene

rubber accelerators. *Rubber Chem. Technol.*, 87, 219-238.

Posters presented at international conferences

- 2013
- M. Cassotti, D. Ballabio, V. Consonni, A. Mauri, I.V. Tetko, R. Todeschini. Modelling of acute aquatic toxicity towards *Daphnia magna* using GA-kNN method. *Final Conference of the ECO Project*, Prien am Chiemsee (Germany).
 - T. Ringsted, S. Luecke, L. Poellinger, M. Cassotti, P. L. Andersson. QSAR models on the effect of dioxins and dioxin-like chemicals to human keratinocytes. *Final Conference of the ECO Project*, Prien am Chiemsee (Germany).
 - F. Grisoni, M. Cassotti, R. Todeschini. Reshaped Sequential Replacement algorithm (RSR) for variable selection. *VIII Colloquium Chemiometricum Mediterraneum*, Bevagna (Italy).
 - V. Consonni, D. Ballabio, F. Sahigara, A. Mauri, M. Cassotti, F. Grisoni, R. Todeschini. A comparative study on different methods for applicability domain assessment. *VIII Colloquium Chemiometricum Mediterraneum*, Bevagna (Italy).
- 2012
- F. Grisoni, M. Cassotti, R. Todeschini. Comparison of variable selection methods. *3rd Summer School on Chemoinformatics*, Strasbourg (France).
 - T. Ringsted, E. Giagloglou, D. Ballabio, A. Mauri, M. Cassotti, V. Consonni, R. Todeschini. Read-across methodology in aquatic ecotoxicology and ready biodegradation. *2nd Winter School of the ECO Project*, Madrid (Spain).

Oral communications

- 2015
- QSAR models for acute aquatic toxicity. *Italian Chemometrics Workshop*, Rome (Italy)
- 2014
- A QSAR model for acute aquatic toxicity towards *Daphnia magna*. *16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014)*, Milan (Italy). Awarded as best presentation by a student.
- 2012
- Modelling of acute aquatic toxicity on *Daphnia magna* and fish. *2nd Summer School of the ECO Project*, Verona (Italy).
- 2011
- The SafeRubber Project. *Italian Chemometrics Workshop*, Albano Laziale (Italy).

Attended conferences and courses

- 2015
- Italian Chemometrics Workshop, Rome (Italy).
- 2014
- EuroScience Open Forum (ESOF2014), Copenhagen (Denmark).
 - 16th International Workshop on Quantitative Structure-Activity Relationships in Environmental and Health Sciences (QSAR2014), Milan (Italy).
- 2013
- Copenhagen School of Chemometrics, Copenhagen (Denmark).
 - Final Conference of the ECO Project, Prien am Chiemsee (Germany).
 - VIII Colloquium Chemiometricum Mediterraneum, Bevagna (Italy).
- 2012
- 3rd Summer School on Chemoinformatics, Strasbourg (France).
 - 2nd Summer School of the ECO Project, Verona (Italy).
- 2011
- Italian Chemometrics Workshop, Albano Laziale (Italy).
 - Orchestra Course and Workshop, Milan (Italy).
 - School of Chemometrics Methods for Process Monitoring, Modena (Italy).
- 2008
- Italian Chemometrics Workshop, Pisa (Italy).

Supervision

2012 Co-supervisor for MSc thesis of Francesca Grisoni. Thesis title: Study of variable selection methods and regression methods for the development of QSAR models for environmental and toxicological endpoints.

Referee activity

- Chemosphere
- SAR and QSAR in Environmental Research
- Iranian Journal of Science and Technology

Interests

Sports I believe in the Roman saying "*mens sana in corpore sano*" (a healthy mind in a healthy body) and, therefore, I like to practice sport. I enjoy windsurfing, skiing, running, motorbike riding and sailing.

Social life I enjoy spending time together with my girlfriend and friends to taste food, have a drink, cook, practice sport and travel.

Arts I like "classical" art, especially gothic, Roman and Greek architecture, and impressionistic painters. I also appreciate modern architecture characterized by state-of-the-art materials and futuristic designs.

Personal information

Date of birth 19/08/1985

Nationality Italian.

Gender Male.

Driving licenses A type
B type