PERSONAL INFORMATION

Viviana Consonni

P.za della Scienza 1, 20126 Milano, Italia

+39 02 64482818 +39 389 1107256

viviana.consonni@unimib.it

http://michem.disat.unimib.it/chm/

Sex Female | Date of birth 28/03/1972 | Nationality Italian

WORK EXPERIENCE

2007 – present

Full researcher

Dept. of Earth and Environmental Sciences, University of Milano-Bicocca, Milano, Italy (http://www.unimib.it)

- Researcher in multivariate data analysis, QSAR, molecular descriptors, similarity analysis; teacher of laboratory courses in analytical chemistry; supervisor of undergraduate, graduate, and PhD students.

2000 - 2017

Scientific consultant

- Scientific consultancy for REACH&Colours Italia s.r.l. (2014-2017), intended to study the relationships between molecular structure and tox/eco-tox/phys-chem properties of dyes.
- Scientific consultancy for Ruffino s.r.l. (2013-2017), intended to provide advanced statistical tools for the geographical origin identification of red wines by ICP-MS elemental analysis.
- Scientific consultancy for Athlon Car Lease Italy s.r.l. (2016), intended to develop multivariate statistical models for the analysis of car price in relation to different marketing scenarios.
- Scientific consultancy for Total Marketing Service France (2014-2015), intended to apply QSPR methods to evaluate the relationships between molecular structure and lubrication properties of gasoil additives.
- Scientific consultancy and training course for ENI S.p.A. (2013) on the use of statistical modelling methods to characterize raw oils through analytical-chemical profiles.
- Training course for Demetra s.r.l. (2013) on statistic-mathematical methods for the analysis of electronic nose-detected chemical data.
- Scientific consultancy for Talete s.r.l. (2000-2007) for the development of DRAGON software for the calculation of molecular descriptors and MOBYDIGS software for the calculation of regression models by using genetic algorithms for variable selection.
- Scientific consultancy for Lusochimica S.p.A. (2005), intended to optimize the rate of a reaction by experimental design methods.
- Scientific consultancy for Lever Fabergé Italia S.p.A. (2004-2005), intended to perform a sensory analysis of tooth pastes. The analysis of the data provided by Lever fabergé on different panel test (QDA e FAT) for the sensory analysis was aimed to evaluate the amount of information available in the data, the significance of the results obtained by QDA and FAT panels, to search for relevant and significant relationships between sensory evaluations and product formulation.
- Scientific consultancy for Bracco S.p.A. (2003), intended to develop methods for image analysis in order to distinguish between noise and signal, identify and detect (pattern recognition) the progression grade of the area affected by pathology.

2001 - 2005

Graduate research assistant

Dept. of Earth and Environmental Sciences, University of Milano-Bicocca, Milano, Italy (http://www.unimib.it).

- Postdoc with a research in chemometrics and QSAR.
- Visiting researcher, School of Mathematical and Physical Sciences, James Cook University of North Queensland (2002).

Business or sector R&D; education

EDUCATION AND TRAINING

1997 – 2000

Ph.D. in Chemical Sciences

University of Siena, Italy

- Doctoral thesis: *Chemometric Methods for Environmental Data Analysis*.
  Supervisor: Prof. Roberto Todeschini

1991 – 1996

B.S. in Environmental Sciences

University of Milano, Italy

PERSONAL SKILLS

Mother tongue(s): Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	Independent	Independent	Good	Good	Independent

Communication skills

- Good communication skills gained through my experience in teaching.

Organisational / managerial skills

- Good organisational / managerial skills gained through my experience as laboratory course instructor, research assistant for a team of 6 people, and project manager.

Job-related skills

- Extensive knowledge of multivariate statistics applied to complex data sets, including several methodologies to extract the relevant information from experimental data. Wide experience in the methodologies intended to face on high complex problems, characterized by presence of noise, absence of specific theories able to predict the evolvement or the outcome of the system under investigation, information related to a huge number of variables, correlation and redundancy of variables together with the impossible a priori discrimination between relevant and useless information for the system.
- Extensive knowledge of molecular descriptors (i.e., numbers extracted by a well defined algorithm from a molecular representation of the molecule) and QSAR (Quantitative Structure-Activity Relationships) techniques.
- Good knowledge of the experimental design methodologies for the research planning, intended to develop a valid experimental design in order to achieve experimental data with a satisfactory amount of information to solve the problem under study. Competence in identifying the optimal working conditions which lead, by further data elaboration, to the problem solution. Experimental design, in effect, covers several techniques to plan a set of informative experiments by using as few experiments as possible thus minimizing costs and time.
- Good expertise in the strategies which support multicriteria decision making processes. Since the criteria can be conflicting, to find an overall optimum that can deviate from the optima of one or more of the single criteria, the ranking requires an aggregation of the criteria expressed mathematically and with the weight assigned to them in the decision process.

Computer skills

- Excellent knowledge of Microsoft Office and the main statistical software: Statistica, SPSS, Unscramble and MATLAB.
- Co-author of MOBYDIGS, software package for the calculation of multivariate regression models by using genetic algorithms (http://www.talete.mi.it).
- Co-author of DRAGON, software package for the calculation of molecular descriptors (https://chm.kode-solutions.net/products_dragon.php).
- Good capacity to perform research in databases. Confidence with the main databases used in the chemical field: SciFinder Scholar, Current Contents, ChemFinder, Sigma-Aldrich, CAS, Chemical Abstracts Service Home Page, NCI-3D Database, ChemIDplus System, NIST Chemistry, IUCLID (International Uniform ChemicaL Database). Experience in simple and advanced queries in SQL on IUCLID database, the database program developed to fulfil European requirements for the evaluation and control of the risks of existing chemical substances.

Other skills

- Good skills in organisation of travels and events.

Driving licence

- B

ADDITIONAL INFORMATION

Publications

Co-author of two books:

- Handbook of Molecular Descriptors, by R. Todeschini and V. Consonni; Wiley-VCH, 2000.
- Molecular Descriptors for Chemoinformatics, by R. Todeschini and V. Consonni; Wiley-VCH, 2009.

Co-author of more than 40 publications in international peer-reviewed scientific journals.

Projects

Partner of EC-funded projects:

- A safer alternative replacement for thiourea based accelerators in the production process of chloroprene rubber (SafeRubber), Grant agreement no.: 2-243756, Funded by the European Community, Call: SME-2008 (2010-2013). Principal investigator: Dr. Claudio Celata (Assocomaplast). Role in the project: project manager of the unit and research assistant.
- Environmental ChemOinformatics (ECO), Grant agreement no.: 238701, Funded by the European Community: Marie Curie Initial Training Networks, Call: FP7-PEOPLE-ITN-2008 (2009-2013). Principal investigator: Dr. Igor Tetko. Role in the project: project manager of the unit and co-supervisor of long-term and short-term fellows.
- Virtual Computational Chemistry Laboratory (VCC-LAB)", INTAS Grant: 00-0363 (2001 – 2004), Coordinator: Dr. Igor Tetko. Role in the project: research assistant.
- Virtual Institute for Chemometrics and Industrial Metrology (VICIM), Project No: GTC1-2002-43030, Contract No.: G7RT-CT-2001-05067, Coordinator: Prof. Luc Massart. Role in the project: research assistant.

Partner of Italian projects:

- Modellazione del processo di formulazione e sviluppo di nuovi prodotti per il settore cosmetico, Programma Regionale DRIADE, Azione DAFNE (2010 – 2011), Scientific coordinator: Prof. Roberto Todeschini. Role in the project: lecturer in the professional training course "Metodologia della Ricerca Sperimentale".
- Sviluppo di strumenti chemoinformatici per la selezione ed identificazione di composti Persistenti Bioaccumulabili e Tossici (PBT) ed Interferenti Endocrini (EDs) nell'ambito del Regolamento REACH, PRIN 2007 (MIUR e Università di Milano-Bicocca), codice 2007R57KT7 (2008 – 2010), Scientific coordinator: Prof. Roberto Todeschini. Role in the project: project manager of the unit and research assistant.

Honours and awards

Best poster award, Conferentia Chemometrica 2011, Sűmeg, Ungheria, 18-21/09/2011

Elected member of the International Academy of Mathematical Chemistry, 2009 (http://www.iamc-online.org)

Designated member of the Editorial Advisory Board of IGI Book Series "Advances in Chemoinformatics and Computational Methods (ACCM)", IGI Global Publishers, 2008 (http://www.igi-global.com/book-series/advances-chemoinformatics-computational-methods-accm/37166)

Award for distinguished young investigators, International Academy of Mathematical Chemistry, 2005 (http://www.iamc-online.org/awards/index.htm)

Memberships

Member of the International Academy of Mathematical Chemistry

Member of the Italian Chemometric Society

Member of Società Chimica Italiana

ANNEXES

List of relevant publications

Ballabio, D., Biganzoli, F., Todeschini, R., Consonni, V. (2017) Qualitative consensus of QSAR ready biodegradability predictions. *Toxicological & Environmental Chemistry*, **99**, 1193-1216.

Royas, C., Todeschini, R., Ballabio, D., Mauri, A., Consonni, V., Tripaldi, P., Grisoni, F. (2017) A QSTR-based Expert System to Predict Sweetness of Molecules. *Frontiers in Chemistry*, **5**, 53.

Grisoni, F., Reker, D., Schneider, P., Friedrich, L., Consonni, V., Todeschini, R., Koeberle, A., Werz, O., Schneider, G. (2017). Matrix-based molecular descriptors for prospective virtual compound screening. *Molecular Informatics*, **36**.

Mauri, A., Ballabio, D., Todeschini, R., Consonni, V. (2016). Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. *Journal of Cheminformatics*, **8:49**, 1-3.

Todeschini, R., Ballabio, D., Grisoni, F., Consonni, V. (2016). A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. *Chemometrics and Intelligent Laboratory Systems*, **157**, 50-57.

Nembri, S., Grisoni, F., Consonni, V., Todeschini, R. (2016). In silico prediction of Cytochrome P450 - Drug interaction: QSARs for CYP3A4 and CYP2C9. *International Journal of Molecular Sciences*, **17**, 914.

Grisoni, F., Consonni, V., Vighi, M., Villa, S., Todeschini, R. (2016). Expert QSAR system for predicting the bioconcentration factor under the REACH regulation. *Environmental Research*, **148**, 507-512.

Mauri, A., Consonni, V., Todeschini, R. (2016). Molecular Descriptors, book chapter in *Handbook of Computational Chemistry*, Springer.

Rojas, C., Ballabio, D., Consonni, V., Tripaldi, P., Mauri, A., Todeschini, R. (2016).Quantitative structure-activity relationships to predict sweet and non-sweet tastes. *Theoretical Chemistry Accounts*, **135**, 66.

Grisoni, F., Consonni, V., Vighi, M., Villa, S., Todeschini, R. (2016). Investigating the mechanisms of bioconcentration through QSAR classification trees. *Environment International*, **88**, 198-205.

Todeschini, R., Ballabio, D., Cassotti, M., Consonni, V. (2015). N3 and BNN: Two new similarity based classification methods in comparison with other classifiers. *Journal of Chemical Information and Modeling*, **55**, 2365-2374.

Grisoni, F., Consonni, V., Nembri, S., Todeschini, R. (2015). How to weight Hasse matrices and reduce incomparabilities. *Chemometrics and Intelligent Laboratory Systems*, **147**, 95-104.

R. Todeschini, D. Ballabio, V. Consonni (2015) Distances and other dissimilarity measures in chemometrics, in Encyclopedia of Analytical Chemistry, ed. Meyers, R.A., John Wiley & Sons.

Cassotti, M., Ballabio, D., Todeschini, R., Consonni, V. (2015) A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (Pimephales promelas). *SAR and QSAR in Environmental Research*, **26**, 217-243.

Grisoni, F., Consonni, V., Villa, S., Vighi, M., Todeschini, R. (2015) QSAR models for bioconcentration: is the increase in the complexity justified by more accurate predictions? *Chemosphere*, 127, 171-179.

Gómez-Carracedo, M.P., Andrade, J.M., Ballabio, D., Prada-Rodríguez, D., Muniategui-Lorenzo, S., Consonni, V., Piñeiro-Iglesias, M., López-Mahía, P., (2015). Impact of medium-distance pollution sources

in a Galician suburban site (NW Iberian peninsula). *Science of the Total Environment*, **512-513**, 114-124.

Cassotti, M., Consonni, V., Mauri, A., Ballabio, D. (2014) Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards Daphnia Magna. *SAR and QSAR in Environmental Research*, **25**, 1013-1036.

Chavan, S., Nicholls, I., Karlsson, B., Rosengren, A., Ballabio, D., Consonni, V., Todeschini, R. (2014) Towards global QSAR model building for acute toxicity: Munro database case study. *International Journal of Molecular Sciences*, **15**, 18162-18174.

Buscema, M., Consonni, V., Ballabio, D., Mauri, A., Massini, G., Breda, M., Todeschini, R. (2014) K-CM: a new artificial neural network. Application to supervised pattern recognition. *Chemometrics and Intelligent Laboratory Systems*, **138**, 110-119.

Ballabio, D., Consonni, V., Mauri, A., Claeys-Bruno, M., Sergent, M., Todeschini, R. (2014) A novel variable reduction method adapted from space-filling designs. *Chemometrics and Intelligent Laboratory Systems*, **136**, 147-154.

Sahigara, F., Ballabio, D., Todeschini, R., Consonni, V. (2014). Assessing the validity of QSARs for ready biodegradability of chemicals: An Applicability Domain perspective. *Current Computer-Aided Drug Design*, **10**, 137-147.

Cherkasov, A., Muratov, E., Fourches, D., Varnek, A., Baskin, I., Cronin, M. T. D., Dearden, J., Gramatica, P., Martin, Y. C., Todeschini, R., Consonni, V., Kuz'min, V., Cramer, R., Benigni, R., Yang, C., Richrad, A., Terfloth, L., Gasteiger, J. and Tropsha, A. (2014). QSAR Modeling: Where have you been? Where are you going to? *Journal Medicinal Chemistry*, **57**, 4977–5010.

Todeschini, R., Consonni, V., Ballabio, D., Mauri, A., Cassotti, M. Lee, S., West, A., Cartlidge, D. (2014). QSPR study of rheological and mechanical properties of Chloroprene rubber accelerators. *Rubber Chemistry and Technology*, **87**, 219-238.

Cassotti, M., Ballabio, D., Consonni, V., Mauri, A., Tetko, I., Todeschini, R. (2014). Prediction of acute aquatic toxicity toward *daphnia magna* by using the GA-*k*NN method. *ATLA: Alternatives to Laboratory Animals*, **42**, 31-41.

Ballabio, D. and Consonni, V. (2013) Classification tools in chemistry. Part 1: Linear models. PLS-DA. *Analitycal Methods*, **5**, 3790-3798.

Mansouri, K., Ringsted, T., Ballabio, D., Todeschini, R. and Consonni, V. (2013) QSAR models for ready biodegradability of chemicals. *Journal of Chemical Information and Modeling*, **53**, 867-878.

Perrone, M. G., Gualtieri, M., Consonni, V., Ferrero, L., Sangiorgi, G. M. L., Longhin, E. M., Ballabio, D., Bolzacchini, E. and Camatini, M. (2013) Particle size, chemical composition, seasons of the year and urban, rural or remote site origins as determinants of biological effects of particulate matter on pulmonary cells. *Environmental Pollution*, **176**, 215-227.

Sahigara, F., Ballabio, D., Todeschini, R. and Consonni, V. (2013) Defining a novel k-Nearest Neighbours approach to assess the applicability of a QSAR model for reliable predictions. *Journal of Chemoinformatics*, **5**, 27-36.

Todeschini, R., Ballabio, D., Consonni, V., Sahigara, F. and Filzmoser, P. (2013) Locally-centred Mahalanobis distance: a new distance measure with salient features towards outlier detection. *Anal. Chim. Acta*, **787**, 1-9.

Ballabio, D., Consonni, V. and Costa, F. (2012) Relationships between apple texture and rheological parameters by means of multivariate analysis. *Chemometrics & Intell. Lab. Syst.*, **111**, 28-33.

Consonni, V. and Todeschini, R. (2012) New similarity coefficients for binary data. *MATCH Commun. Math. Comput. Chem.*, **68**, 581-592.

Consonni, V. and Todeschini, R. (2012) Multivariate Analysis of Molecular Descriptors, in *Statistical Modelling of Molecular Descriptors in QSAR/QSPR* (eds. M. Dehmer, K. Varmuza and D. Bonchev), Wiley-Blackwell, Weinheim (Germany), pp. 111-147.

Mansouri, K., Consonni, V., Durjava, M. K., Kolar, B., Öberg, T. and Todeschini, R. (2012) Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. *Chemosphere*, **89**, 433-444.

Sahigara, F., Mansouri, K., Ballabio, D., Mauri, A., Consonni, V. and Todeschini, R. (2012) Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. *Molecules*, **17**, 4791-4810.

Todeschini, R., Consonni, V., Xiang, H., Holliday, J., Buscema, M. and Willett, P. (2012) Similarity

coefficients for binary chemoinformatics data: overview and extended comparison using simulated and real datasets. *Journal of Chemical Information and Modeling*, **52**, 2884-2901.

Fernandez-Varela, R., Gomez-Carracedo, M. P., Ballabio, D., Andrade, J. M., Consonni, V. and Todeschini, R. (2010) Self Organizing Maps For Analysis Of Polycyclic Aromatic Hydrocarbons 3-Way Data From Spilled Oils. *Analytical Chemistry*, **82**, 4264-4271.

Consonni, V., Ballabio, D. and Todeschini, R. (2009) Comments on the definition of the Q^2 parameter for QSAR validation. *Journal of Chemical Information and Modeling*, **49**, 1669-1678.

Todeschini, R. and Consonni, V. (2009) *Molecular Descriptors for Chemoinformatics (2 volumes)*, WILEY-VCH, Weinheim (Germany), 1257 pp.

Consonni, V. and Todeschini, R. (2008) New Spectral Indices for Molecule Description. *MATCH*, **60**, 3-14.

Mauri, A., Consonni, V., Pavan, M. and Todeschini, R. (2006) DRAGON software: an easy approach to molecular descriptor calculations. *MATCH*, **56**, 237-248.

Todeschini, R., Consonni, V., Mauri, A. and Pavan, M. (2004) Detecting "bad" regression models: multicriteria fitness functions in regression analysis. *Anal. Chim. Acta*, **515**, 199-208.

Todeschini, R. and Consonni, V. (2003) Descriptors from Molecular Geometry, in *Handbook of Chemoinformatics - Vol.3*, Vol. 3 (ed. J. Gasteiger), WILEY-VCH, Weinheim (GER), pp. 1004-1033.

Consonni, V., Todeschini, R., Pavan, M. and Gramatica, P. (2002) Structure/Response Correlations and Similarity/Diversity Analysis by GETAWAY Descriptors. 2. Application of the Novel 3D Molecular Descriptors to QSAR/QSPR Studies. *Journal of Chemical Information and Computer Sciences*, **42**, 693-705.

Consonni, V., Todeschini, R. and Pavan, M. (2002) Structure/Response Correlations and Similarity/Diversity Analysis by GETAWAY Descriptors. 1. Theory of the Novel 3D Molecular Descriptors. *Journal of Chemical Information and Computer Sciences*, **42**, 682-692.